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THEORY OF ULTRASONIC PULSE MEASUREMENTS OF THIRD ORDER ELASTIC CONSTANTS FOR CUBIC CRYSTALS

A THESIS

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SUMMARY

The purpose of the research reported in this thesis is to obtain some theoretical results needed for the development of two new experiments for measuring the third order elastic constants of solids. The particular solids considered are crystals having cubic symmetry, but most of the results can be generalized to other symmetry classes.

The first experiment considered is the wave distortion experiment, which measures the distortion of an initially sinusoidal wave propagating in the solid. The distortion can be measured by making a Fourier analysis of the wave after it has propagated through a sample of the material being investigated and the present investigation shows that the amplitudes of the fundamental and second harmonic frequency components of the distorted wave can be used to calculate a value for a linear combination of the third order elastic constants of the solid. The particular linear combination measured will depend on the propagation and polarization directions of the input wave, so that an important part of the investigation was to relate the propagation and polarization directions to the particular linear combination of the third order elastic constants obtainable. The relationship which was found to exist is algebraically very complicated and, as such, is of very little use to one who would like to do the experiment. In order to present the relationships in a useful form, a set of tables was made with the help of a digital computer. These tables list the obtainable linear combinations of third order elastic constants as a function of propagation and polari-

zation directions for six particular materials.

It is shown that, for cubic crystals, this type of experiment is capable of measuring values for enough linear combinations of elastic constants to determine values for C_{111}, C_{112}, C_{166}, $(2\,C_{144} + C_{123})$, and $(\frac{1}{2}\,C_{144} + C_{456})$. In order to estimate the error one could expect in these values, some calculations based on elastic constants measured by other methods are used to try to find out how the experimental uncertainty would be reflected in the uncertainty in the calculated values of the elastic constants. These calculations suggest that there would be large relative uncertainties in the calculated values of $(2\,C_{144} + C_{123})$ and $(\frac{1}{2}\,C_{144} + C_{456})$.

Two questions are considered in connection with the manner in which the experiment is to be performed. First, one would like to know whether or not the distortion of the wave will continue after reflection from a stress-free boundary. This question is important because the experimentally observed distortion is very small, but increases with path length. If the distortion continued after reflection from the end of the sample of the material, then a long propagation distance could be observed in a short sample by utilization of several transits. The equations of motion were solved on a computer with the result that the wave would, in fact, begin to undistort after reflection; so that it would not be possible to utilize several transits of the sample. A qualitative argument is given to support this result.

The second of these questions affects the geometry of the experiment. Previous investigations have shown that a plane wave of finite extent will travel in the energy flux direction rather than the propa-

gation direction. Since the experiment will actually be done with a finite plane wave, the present report undertakes to show how the wave generator and detector can be positioned on the sample to account for the deviation of the energy flux direction from the propagation direction.

Because the wave distortion experiment cannot be used to measure all six third order elastic constants of cubic crystals, another experiment was considered. This experiment measures the amplitude of a scattered wave produced by the interaction of two intersecting non-collinear ultrasonic beams propagating in the solid. Quantum mechanical time dependent perturbation theory is used to show that if one measures the amplitudes of the input and scattered waves, along with the geometrical parameters of the experiment, then he can calculate a value for a linear combination of third order elastic constants of the solid. As in the wave distortion experiment, the particular combination measured depends on the propagation and polarization directions used; but for the scattering experiment enough combinations can be obtained to determine all six of the third order constants.

The expression relating the wave amplitudes to the elastic constants is valid only for resonant interactions; that is, interactions for which the conservation laws for energy and momentum are satisfied. These conservation laws take the form of complicated algebraic equations, so that the derived expression for calculating the elastic constants is of little value without the specification of some useful resonant interactions. A method of successive approximations which can be used to find resonant interactions has been developed and utilized to find some potentially useful interactions for measuring elastic constants. Tables

are given which list enough interactions, for six particular materials, to allow one to find values for all of the third order elastic constants except C_{111}. This quantity has been regarded as known since it is conveniently measured by the wave distortion experiment.

CHAPTER I

INTRODUCTION

The research reported here is an investigation of some theoretical problems involved in two experiments proposed for measuring the third order elastic constants of cubic crystals. Since there are two experiments, the research is divided into two distinct parts which are described in the second and third chapters of this thesis. The respective chapters contain the statements of the problems investigated, the conclusions, and the recommendations; so that the reader who has an interest in only one of the experiments can conveniently ignore the other.

This introductory chapter is also organized for the convenience of such a reader. The first section is devoted to motivation, which is common to all of the work done. The second and third sections give brief descriptions of the two experiments which were investigated, along with a brief history and a review of the literature for each.

1. Motivation

Many solid state phenomena can be described by means of a model (1) which views a crystal lattice as a collection of point masses, each of which is interconnected by a collection of massless springs. The elastic potential energy of this model can be expanded in a Taylor series about the equilibrium configuration of the lattice, where the independent variables for the expansion are the coordinates of the displacement vectors of the individual point masses. The coefficients of

the terms in the expansion are called the microscopic coupling parameters and, if one could measure them, then he could describe all of the properties of the lattice. In principle, one could measure the microscopic coupling parameters if he could generate sound waves with wavelengths comparable to the lattice spacing. Unfortunately, the maximum frequency of sound waves presently obtained in the laboratory falls short of this goal by several orders of magnitude.

Propagation of ultrasonic waves of frequencies currently attainable in the laboratory is described by means of the continuum model of the solid. In this case, the elastic potential energy density is expanded in a Taylor series in the strain coordinates and the coefficients, the elastic constants,can be measured in the laboratory. Although the elastic constants are not as basic to a knowledge of the forces in the lattice as the coupling parameters, they have proved useful in predicting many microscopic effects (2-3). Further, one can predict the values of the elastic constants for single crystals by means of a theoretical model which calculates the forces between the lattice points (4-6); thus, comparing the predicted values of the elastic constants with the measured ones will provide a check of the theoretical predictions of the lattice forces.

Since the potential energy is expanded about the equilibrium configuration, a first approximation is obtained by retaining only quadratic strain terms, whose coefficients are the second order elastic constants. This approximation describes a harmonic solid and is adequate for describing many physical phenomena. However, other phenomena require the consideration of the higher order terms for their description (7).

Examples are thermal expansion, thermal conductivity, phonon-lattice defect interactions, high temperature specific heat, the variation of the normal mode frequencies with volume, and the phonon-phonon interactions leading to thermal equilibrium. The existence of these phonomena makes a knowledge of the values of the higher order elastic constants very important.

One may gain a knowledge of the lowest order anharmonic effects by measuring the third order elastic constants and, in fact, considerable progress has been made in this direction in the past few years. One method has been developed which will determine a complete set of third order elastic constants for cubic crystals (8) and, since 1961, values have been published for at least six materials (9-12). In addition to the presently successful techniques for measuring the third order elastic constants, several new methods are being developed (13-14). The purpose of the research reported in this thesis is to obtain some theoretical results needed for the development of two of these new experiments.

2. Ultrasonic Wave Distortion Experiments

The first of these two experiments utilizes the fact that an initially sinusoidal plane wave propagating through a solid will undergo progressive distortion as it propagates. This fact was first demonstrated experimentally by Gedroits and Krasil'nikov (15) at the Moscow State University. In 1962, they reported observing the progressive generation of a 10 megacycle Fourier component in an initially pure 5 megacycle sound wave propagating in a magnesium-aluminum alloy. In 1963, Breazeale and Thompson (16) at Oak Ridge National Laboratory reported analogous observations for 30 megacycle sound waves in polycrystal-

line aluminum.

Results of continued study of these experiments were published by Breazeale and Ford (17) in 1965. They established that for a typical experiment the distortion of the wave can be represented as a linear increase of the second harmonic Fourier component with distance traveled. In addition, they related this rate of increase of second harmonic content to linear combinations of third order elastic constants for the special cases of longitudinal waves traveling in the [100], [110], and [111] directions in cubic crystals.

In all of these first studies of the experiment, the detection and measurement of the distorted wave was accomplished by means of a piezo-electric crystal transducer which converts the mechanical vibration to an electric signal. Such a detector is useful for making relative amplitude measurements, but for measuring elastic constants one needs to measure absolute amplitudes of the fundamental and second harmonic components of the wave. To this end, Gauster and Breazeale (18) developed a capacitive detector which is capable of measuring amplitudes of longitudinal waves in the frequency range from 5 to 100 megacycles. Because this device is limited to detection of longitudinal waves, another device, such as that suggested by Michailov (19), will need to be developed for measurements for other polarizations.

In anticipation of this development, the present study sought to relate linear combinations of third order elastic constants to measurable quantities for directions other than the three special cases already considered. It was desired to know which directions yield useful linear combinations of third order elastic constants and, finally, to know

whether enough linear combinations could be obtained to permit one to determine all six third order elastic constants for cubic materials.

3. Beam Scattering Experiments

One result of the study of wave harmonic distortion experiments was that the method could not yield enough information to permit calculation of all six third order elastic constants (20). To remedy this deficiency, a second experiment was considered. This experiment utilizes the fact that two intersecting, large amplitude sound waves can interact to produce a scattered wave whose amplitude will be a function of the higher order elastic constants of the solid.

A complete discussion of the use of third order elastic constants in the description of interacting sound waves was given by Ziman (1) in 1960. His quantum mechanical discussion shows that the conservation laws for energy and momentum determine the interaction geometries which will produce a scattered wave. In addition, he demonstrates that one can use the nonlinear terms in the elastic potential energy expression to calculate a quantum mechanical transition probability by means of time dependent perturbation theory.

In 1963, Jones and Kobett (21) published a paper which predicts the amplitude of the scattered wave produced by the interaction of two infinite plane waves propagating in an isotropic solid. Their classical treatment results in resonance conditions, analogous to the quantum mechanical conservation laws, which define the bounds on the interaction geometries. In 1964, Childress and Hambrick (22) gave a treatment of the same problem which uses a wave packet formalism instead of infinite

plane waves.

Later in 1964, Taylor and Rollins (23) published a paper in which elasticity theory is treated quantum mechanically for the case of interactions in isotropic solids. Their work, which also predicts scattered wave amplitudes and selection rules for allowed interactions, agrees with the classical theory of Jones and Kobett, but requires considerably fewer algebraic manipulations. In a companion paper, Rollins, Taylor, and Todd (24) report experimental observation of the scattered wave and verification of the predictions of the selection rules for resonant scattering. Since they used transducers to detect the scattered wave, there was no way to obtain absolute amplitude measurements and hence they were not able to check the predictions of scattered wave amplitude.

Since these reports were made, a capacitive detector has been developed by Gauster and Breazeale (18). This device enables one to measure the absolute amplitude of longitudinal ultrasonic waves, so that it should now be possible to check the theoretical predictions of scattered wave amplitude. If a means for making absolute amplitude measurements for other polarizations (19) is developed, then these experiments can be useful for measuring the higher order elastic constants of single crystals.

In order to help make this possible, the present study applied the quantized elasticity theory to the problem of ultrasonic beam scattering in anisotropic solids. Using an argument analogous to that of Taylor and Rollins, perturbation theory is used to find an expression for the amplitude of the scattered wave as a function of the amplitudes of the input waves and a linear combination of the third order elastic constants. A value for this linear combination of third order elastic constants can be

calculated from the results of an experiment measuring the amplitude of the input and scattered waves. Since the particular linear combination obtained depends on the interaction one measures, enough different allowed interactions have been suggested to allow one to determine all of the elastic constants except C_{111}. This quantity is conveniently measured by the wave harmonic distortion experiment, so it has been regarded as known for this part of the work.

CHAPTER II

ULTRASONIC WAVE DISTORTION EXPERIMENTS

The purpose of the research described in this chapter is to investigate some theoretical problems involved in a newly developed technique for measuring the third order elastic constants of solids. This technique is based on the fact that an initially sinusoidal sound wave will undergo progressive distortion as it propagates through a solid (15). For a wide range of the experimental parameters the distorted wave can be described as the sum of the original sinusoid plus a second harmonic whose amplitude increases linearly with the propagation distance (17). The amplitude of second harmonic present is proportional to the propagation distance and to a linear combination of second and third order elastic constants. This linear combination of elastic constants depends in turn on the polarization and propagation directions of the sound wave. The object of this chapter then is to calculate the obtainable linear combinations of elastic constants as a function of polarization and propagation directions. This chapter thus provides the experimentalist with the information needed to calculate third order elastic constants from measured harmonic distortion data.

The first section of the chapter presents the elasticity theory necessary for the calculations (25). In it, the elastic continuum model used for describing the single crystal is discussed and the equations of motion for large amplitude sound waves in the crystal are derived. The

equations of motion are then reduced to a simplified form in which the relevant linear combination of elastic constants appears as a coefficient. The second section of the chapter is devoted to solving the problem of determining how many independent linear combinations of the elastic constants appear in the simplified equations of motion when the polarization and propagation directions are varied.

Section three tabulates the linear combination of third order elastic constants as a function of propagation and polarization directions. These tables, which are designed to enable one who wishes to do the experiment to choose useful directions by his own criteria, are given for copper, gold, silicon, germanium, sodium chloride, and potassium chloride. A sample calculation is presented which allows one to estimate the uncertainties to be expected in values of the elastic constants calculated from the wave distortion data.

The fourth section of the chapter presents a consideration of how the geometry of the experiment is affected by the deviation of the energy flux direction from the propagation direction.

Since the work described in this thesis is in two disjoint parts, the concluding remarks and results for this portion of the research are given at the end of this chapter instead of at the end of the thesis.

1. Equations of Motion

This section begins with a discussion of the mathematical model used to describe large amplitude sound waves in an anistropic solid. Then the equations of motion are derived and reduced to a form suitable for the description of plane wave propagation. Finally, the approximate

solution of the plane wave equation of motion is given along with a consideration of the behavior of the wave after a reflection.

The Mathematical Model

Since the wave lengths of the pulses being studied here are much larger than the lattice spacings in the crystal and since we choose to neglect the effect of attenuation, for the purpose of this work a solid is taken to be a nondispersive, perfectly elastic continuum. The continnum is taken to include anisotropic effects because single crystal samples are to be investigated; and, since high frequencies and large amplitudes are involved, Murnaghan's finite deformation elasticity theory (25) is used. Finite deformation elasticity theory discards the assumption, used in the infinitesimal theory, that in the elastic energy the powers of the displacement coordinates greater than the second may be neglected. Discarding this assumption necessitates a more general definition of the strain tensor and the use of more general equations of motion.

For finite deformations the strain tensor is defined by the relation (25)

$$\eta_{ij} = \frac{1}{2}\left(\sum_{k=1}^{3} \frac{\partial x_k}{\partial a_i}\frac{\partial x_k}{\partial a_j} - \delta_{ij}\right) \quad , \tag{1}$$

where δ_{ij} is the Kronecker δ and the symbols i and j take on the values 1, 2, 3 . In Equation (1) the a_i are the cartesian coordinates of a point of the continuum in the unstrained state. The vector x_i represents the cartesian coordinates of the same point at time t, i.e., in the deformed state. Here a_i and t are independent variables upon which the

variables x_i depend. One writes

$$x_i = x_i(a_1, a_2, a_3, t) \quad , \tag{2}$$

where i takes on the values 1, 2, 3 . Several comments about η are in order. First, η is symmetric by inspection; second, the definition of η does not require that the coordinate systems for a_i and x_i coincide; and third, Murnaghan (25) has shown that the coordinates of η transform as a second order tensor with respect to rotations of the a_i coordinate axes while the coordinates of η are invariant under rotations of the x_i coordinate axes.

The description of the mathematical model is completed by the assumption that the elastic potential energy density (per unit unstrained volume) of the continuum is

$$\Phi = \frac{1}{2!} \sum_{\substack{i,j,k,\ell \\ = 1}}^{3} C_{ijk\ell}\, \eta_{ij}\, \eta_{k\ell} + \frac{1}{3!} \sum_{\substack{m,n,p,q,r,s \\ = 1}}^{3} C_{mnpqrs}\, \eta_{pq}\, \eta_{rs}\, \eta_{mn} \, . \tag{3}$$

Note that this expression goes one term beyond the infinitesimal theory by including terms cubic in the strain coordinates. Here the coordinate axes are taken to coincide with the symmetry axes of the crystal so that $C_{ijk\ell}$ and C_{mnpqrs} are the usual second and third order elastic constants as defined by Brugger (26). Birch (27) has shown that the symmetry requirements for various classes of crystals imply that only certain of the $C_{ijk\ell}$ and C_{mnpqrs} are non-zero and distinct. For crystals of cubic symmetry, Equation (3) can be rewritten

$$\Phi(\eta) = \frac{1}{2} C_{11}(\eta_{11}^2 + \eta_{22}^2 + \eta_{33}^2) + 2 C_{44}(\eta_{12}^2 + \eta_{31}^2 + \eta_{23}^2) \qquad (4)$$

$$+ C_{12}(\eta_{11}\eta_{22} + \eta_{11}\eta_{33} + \eta_{22}\eta_{33}) + \frac{1}{6} C_{111}(\eta_{11}^3 + \eta_{22}^3 + \eta_{33}^3)$$

$$+ \frac{1}{2} C_{112}[(\eta_{22} + \eta_{33})\eta_{11}^2 + (\eta_{11} + \eta_{33})\eta_{22}^2 + (\eta_{11} + \eta_{22})\eta_{33}^2]$$

$$+ 2 C_{144}[\eta_{11}\eta_{23}^2 + \eta_{22}\eta_{31}^2 + \eta_{33}\eta_{12}^2]$$

$$+ 2 C_{166}[\eta_{12}^2(\eta_{11} + \eta_{22}) + \eta_{23}^2(\eta_{22} + \eta_{33}) + \eta_{31}^2(\eta_{33} + \eta_{11})]$$

$$+ C_{123}\eta_{11}\eta_{22}\eta_{33} + 8 C_{456}[\eta_{12}\eta_{23}\eta_{31}] \quad .$$

In this expression the number of subscripts on the elastic constants has been reduced by the convention: 11 → 1, 22 → 2, 33 → 3, 12 → 6, 13 → 5, and 23 → 4. Equation (4) differs from Birch's expression by some constant factors because Brugger's notation, which has been used here, is different from that of Birch.

The Equations of Motion

The expression for the elastic potential energy density given by Equation (4) can be used along with Lagrange's equations for continuous media to derive the equations of motion for the anisotropic continuum. For convenience in writing, define the matrix

$$J_{k\ell} = \frac{\partial x_k}{\partial a_\ell} \qquad (5)$$

and let ρ be the unstrained mass density of the continuum. The Lagrangian density of the system can be written

$$L = \frac{1}{2} \sum_{i=1}^{3} \rho \dot{x}_i^2 - \Phi(\eta) \quad , \tag{6}$$

where the dot superscript denotes a time derivative. Lagrange's equations take the form (28)

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) + \sum_{k=1}^{3} \frac{d}{da_k} \frac{\partial L}{\partial\left(\frac{\partial x_i}{\partial a_k}\right)} = 0 \quad , \tag{7}$$

where here and in the following equations i = 1, 2, and 3. Using Equations (6) and (7) one obtains

$$\rho \ddot{x}_i - \sum_{jk\ell} \frac{d}{da_j}\left(\frac{\partial \Phi}{\partial \eta_{k\ell}} \frac{\partial \eta_{k\ell}}{\partial\left(\frac{\partial x_i}{\partial a_j}\right)}\right) = 0 \quad . \tag{8}$$

Differentiating Equation (1) yields

$$\frac{\partial \eta_{k\ell}}{\partial\left(\frac{\partial x_i}{\partial a_j}\right)} = \frac{1}{2} \delta_{jk} \frac{\partial x_i}{\partial a_\ell} + \frac{1}{2} \delta_{j\ell} \frac{\partial x_i}{\partial a_k} \quad , \tag{9}$$

where δ_{jk} is the Kronecker δ. Putting Equation (9) into Equation (8) one obtains the equations of motion in their usual form

$$\rho \ddot{x}_i = \sum_{k=1}^{3} \frac{d}{da_k}\left(\sum_{\ell=1}^{3} J_{i\ell} \frac{\partial \Phi}{\partial \eta_{k\ell}}\right) \quad , \tag{10}$$

where it has been assumed that the potential energy density expression given in Equation (4) has been rewritten so that

$$\frac{\partial \Phi}{\partial \eta_{k\ell}} = \frac{\partial \Phi}{\partial \eta_{\ell k}} \quad , \tag{11}$$

where ℓ and k take on the values 1, 2, 3.

As it stands, Equation (10) is too complicated to be useful for these experiments. If the expression for Φ were substituted into Equation (10) and if the equations were written out in terms of x_i as the dependent variables with a_i and t as independent variables, the resulting equations would be a system of three partial differential equations in four independent variables with nonlinear and linear coupling and with roughly 45 terms in each equation. Fortunately, certain aspects of the experiment to be performed will allow Equation (10) to be simplified. In particular, three things about the experiment permit simplification in the equations of motion. First, the experiment involves only single plane wave pulses. Thus, by judicious choice of coordinate axes, one may reduce the number of independent variables from four to two, namely the time and the distance along the propagation direction. Second, it has been shown that in the range of the parameters being considered many of the nonlinear terms make a negligible contribution to the equations of motion and thus may be dropped. Third, if the polarization direction of the plane wave being considered is properly chosen then the number of dependent variables, and consequently the number of equations, can be reduced to one.

Plane Wave Equations of Motion

In Equation (10), the equations of motion, the orientation of the a_k axes is arbitrary. If the a_1 axis is taken as the propagation direction for an infinite plane wave then Equation (10) can be rewritten

$$\rho \ddot{x}_i = \frac{d}{da_1} \sum_{k=1}^{3} J_{ik} \frac{\partial \Phi(\eta)}{\partial \eta_{1k}} \tag{12}$$

where i = 1, 2, 3 and where η is calculated from Equation (1) by taking the a_1 axis parallel to the propagation direction. The dependent variables in these simplified equations of motion, Equation (12), are independent of a_2 and a_3 because only plane waves are being considered.

However, one must pay a price for this simplification. The elastic constants are defined as coefficients in an expansion of the elastic energy in powers of the strain when the strain is calculated with the a_k axes parallel to the symmetry axes of the crystal. Thus, in order that $\Phi(\eta)$ in Equation (12) contain the usual elastic constants, we must determine the change in Φ and η under a rotation of the a_k axes. To this end, let a bar superscript denote a quantity calculated with the a_k axes parallel to the crystal symmetry axes. Quantities without a bar superscript are calculated with the a_1 axis parallel to the propagation direction.

As mentioned previously, Murnaghan (25) has shown that

$$\bar{\eta} = R^* \eta R \quad , \tag{13}$$

where R is the orthogonal matrix which rotates the $\bar{a}_k$ axes into the a_k axes and where R^* is the transpose of R. Furthermore, since the elastic energy is a scalar under rotations, the expression for Φ can be written

$$\Phi(\eta) = \bar{\Phi}(\bar{\eta}) = \bar{\Phi}(R^* \eta R) \quad ; \tag{14}$$

that is, if

$$\bar{\Phi}(\bar{\eta}) = \frac{C_{11}}{2}\left(\bar{\eta}_{11}\right)^2 + \frac{C_{111}}{6}\left(\bar{\eta}_{11}\right)^3 + \ldots \quad , \tag{15}$$

where C_{ij} and C_{ijk} denote the second and third order elastic constants, then

$$\Phi(\eta) = \frac{C_{11}}{2}\left(\sum_{jk=1}^{3} R^*_{1j}\ \eta_{jk}\ R_{k1}\right)^2 + \frac{C_{111}}{6}\left(\sum_{jk=1}^{3} R^*_{1j}\ \eta_{jk}\ R_{k1}\right)^3 + \ldots . \tag{16}$$

Hence, Equation (12) will contain the usual elastic constants if it is written in the form

$$\rho\ddot{x}_i = \frac{d}{da_1}\left\{\sum_{k=1}^{3} J_{ik}\ \frac{\partial\ \bar{\Phi}\ (R^*\ \eta R)}{\partial\ \bar{\eta}_{1k}}\right\} \quad , \tag{17}$$

where η is the strain calculated taking the a_1 axis along the propagation direction.

Define the coordinates of the displacement vector at a point by the expression

$$u_k = x_k - a_k \quad , \tag{18}$$

where the x_k axes have been taken as coincident with the a_k axes. If Equation (3), symmetrized in accordance with the requirement of Equation (11), is substituted into Equation (17) along with the transformation defined in Equation (18) then the equations of motion become

$$\rho\ u_{i,tt} = \sum_{j=1}^{3} A_{ij}\ u_{j,aa} + \sum_{j,k=1}^{3} B_{ijk}\ u_{j,a}\ u_{k,aa} \quad . \tag{19}$$

In this equation, the notation

$$u_{j,a} = \frac{\partial u_j}{\partial a_1} \ , \ u_{i,tt} = \frac{\partial^2 u_i}{\partial t^2} \ , \text{ and } \ u_{\ell,aa} = \frac{\partial^2 u_\ell}{\partial a_1^2}$$

is used. The A_{ij} are known linear combinations of second order elastic constants and the B_{ijk} are known linear combinations of second and third order elastic constants. Since the u_k depend on only one space variable a_1, the subscript on a_1 has been dropped. Finally, in going from Equation (17) to Equation (19) only the lowest order nonlinear terms have been retained since current experiments measure only this lowest order nonlinearity.

Now Equation (19) is a much manageable form for the equations of motion than is Equation (10). Nonetheless, Equation (19) is defective for the purpose of these experiments in that the three components u_k are linearly coupled via the terms $\sum_{j=1}^{3} A_{ij} u_{j,aa}$. Consequently, new dependent variables P_k are now introduced in order to remove this linear coupling. Since the known coefficients A_{ij} in Equation (19) form a symmetric matrix, there exists an orthogonal matrix S such that $S^* AS$ is diagonal. Hence, if one introduces the transformation

$$u_j = \sum_{k=1}^{3} S_{jk} P_k \tag{20}$$

into Equation (19), he obtains

$$\rho P_{j,tt} = \mu_j P_{j,aa} + \sum_{\ell m=1}^{3} \nu_{j\ell m} P_{\ell,a} P_{m,aa} \ , \tag{21}$$

where μ_j are the eigenvalues of the A_{ij} matrix and where the derivative notation is the same as in Equation (19). The eigenvectors of A_{ij} repre-

sent the polarization directions which are uncoupled in the linear approximation. Thus, P_j is the amplitude corresponding to the jth uncoupled polarization. The $\nu_{j\ell m}$ are known linear combinations of the second and third order elastic constants.

The equations of motion for a plane wave given in Equation (21) are exact through the lowest order nonlinear terms. They may, however, be simplified even further using perturbation theory. The sound wave amplitudes currently available in the laboratory are sufficiently small that the nonlinear terms of Equation (21) may be treated as small perturbations. Moreover, in these experiments one introduces a plane wave sinusoidal pulse into one end of the crystal and then measures only that second harmonic distortion which increases linearly with propagation distance. Now a straightforward perturbation calculation (see Appendix) shows that only those terms in Equation (21) for which $j = \ell = m$, or for which $\ell = m$ and $\mu_j = \mu_\ell$ yield a second harmonic which increases linearly with propagation distance. Such terms are said to be resonant. Those for which $j = \ell = m$ are called self-resonant and those for which $\ell = m$ and $\mu_j = \mu_\ell$ are called mutual-resonant terms. Mutual resonance occurs only if there is an accidental degeneracy, $\mu_j = \mu_\ell$. This degeneracy, depending as it does on propagation direction and second order elastic constants, occurs so infrequently that it will be excluded from the following discussion. Finally, we note that in general the nonresonant terms in Equation (21) lead to second harmonic generation which is smaller, relative to the resonant generation, by several orders of magnitude.

Finally then, the experimentally relevant equations of motion for

a plane wave in a solid take the simple form

$$\rho P_{j,tt} = \mu_j P_{j,aa} + \nu_{jjj} P_{j,a} P_{j,aa} \quad , \tag{22}$$

where $j = 1, 2, 3$. If the generated plane wave is linearly polarized along one of the three independent polarization directions then only one of the three equations given by Equation (22) is nontrivial. The solution of this equation and its use in relating measured quantities to elastic constants are the subjects of the next part of this section.

Solution of the Equation of Motion

Breazeale and Ford (17) have shown that the perturbation solution of Equation (22) given by

$$P_j = B_j \sin(\omega t - k_j a) - (\nu_{jjj}/8\mu_j) B_j^2 k_j^2 a \cos(2\omega t - 2k_j a) \tag{23}$$

is sufficiently accurate to describe the results of wave harmonic distortion experiments. In this equation the angular frequency ω and the wave number k_j are related by the equation $\omega^2 = \frac{\mu_j}{\rho} k_j^2$, and B_j is the amplitude of P_j at $a = 0$. The second harmonic amplitude, H_{2j}, of P_j is given by

$$H_{2j} = - (\nu_{jjj}/8\mu_j) B_j^2 k_j^2 a \quad , \tag{24}$$

where a is the distance through which the initially sinusoidal disturbance has propagated. Thus, if one introduces into one end of a solid a plane sine wave with polarization such that only one component P_j is nonzero, then he may determine the linear combination of second and third order elastic constants ν_{jjj} by putting measured values of H_{2j}, B_j, k_j, and a into Equation (24). The magnitude of H_{2j} is found by measuring the

magnitude of the second harmonic component of the distorted wave and the sign of H_{2j} is found by observing the relative phase of the fundamental and the second harmonic components. Since the second order elastic constants are usually known, determining ν yields a definite value for one linear combination of third order elastic constants.

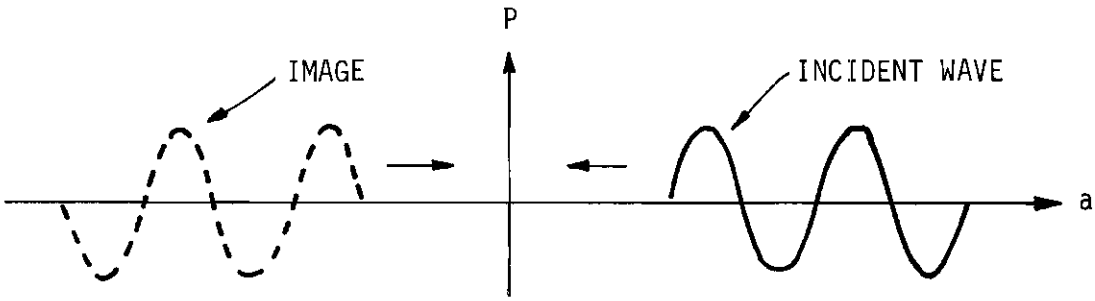
Reflection from a Boundary

A question that arises from the solution of the equation of motion is: does the second harmonic amplitude, H_{2j}, continue to increase after the pulse has been reflected from a stress-free boundary (the end of a crystal sample)? This question is relevant because if the answer were yes then one could cut sample costs and obtain a long path length in the medium by utilizing several transits of the sample.

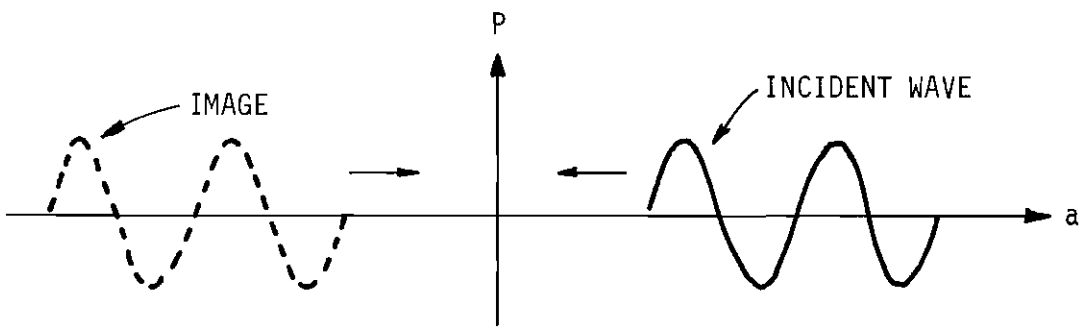
The behavior of a distorted wave after reflection from a boundary can be inferred without reference to the perturbation solution given above. To do this one rewrites Equation (22) in the form

$$\rho P_{tt} = (\mu + \nu P_a) P_{aa} \quad . \tag{25}$$

The subscripts a and t denote partial derivatives and the subscript j has been omitted because we are only considering one polarization. Equation (25) can be thought of as a wave equation for which the phase velocity at a given point in the wave depends on the strain, P_a, at that point. If we suppose, as is usually the case, that $\nu < 0$ then a point traveling with the wave for which $P_a > 0$ will move more slowly than those for which $P_a = 0$ or $P_a < 0$. Conversely, one would expect that points for which $P_a < 0$ will move faster than points for which $P_a = 0$ or $P_a > 0$. This variation of the phase velocity with position on the wave



STRESS-FREE BOUNDARY AT a = 0



FIXED BOUNDARY AT a = 0

Figure 1. Reflection from Stress-free and Fixed Boundaries.

will cause some points to "lag behind" while others will "catch up" and so the wave will distort as it propagates through the solid.

Suppose $P = f(\omega t + ka)$ is a wave which has been distorted and suppose it is reflected from a stress-free boundary at $a = 0$. Figure 1 leads one to expect that after reflection the wave would be represented by

$$P = f(\omega t - ka) \quad . \tag{26}$$

By differentiating Equation (26) one can see that those points for which $P_a > 0$ had been true before the reflection now have $P_a < 0$. Thus, the process of distortion would be reversed and the wave would undistort since points which had "lagged behind" before reflection would now be trying to "catch up."

On the other hand, if the boundary at $a = 0$ had been a fixed boundary then one would expect the reflected wave to have the form

$$P = - f(\omega t - ka) \quad , \tag{27}$$

so that the process of distortion would continue.

In order to substantiate the intuitive argument given above, Equation (25) was solved on a computer by means of a finite difference method. Periodic boundary conditions were used first in order to verify the perturbation solution given in Equation (23). This done, the above predictions concerning reflections from fixed and stress-free boundaries were also verified.

2. Obtainable Linear Combinations

This section of the chapter is concerned with finding out how many

of the third order elastic constants one can measure by means of the wave harmonic distortion experiments. In particular, the equations of motion for a single plane wave in a cubic crystal are shown to depend on the five parameters C_{111},C_{112}, C_{166}, $(2C_{144} + C_{123})$, and $(\frac{1}{2}C_{144} + C_{456})$ instead of all six third order elastic constants. Since the wave harmonic distortion method uses a single plane wave pulse, these five parameters are the only quantities which can be measured by this technique. Computer calculations leading to these conclusions are described in the first part of this section and an analytic proof is given in the second part.

Some Calculations

In Section 1 of this chapter it was shown that by means of the wave harmonic distortion method one could measure a linear combination of second and third order elastic constants, ν. One can write this linear combination as

$$\nu = a_1 C_{111} + a_2 C_{112} + a_3 C_{144} + a_4 C_{166} + a_5 C_{123} + a_6 C_{456} + b_1 C_{11} + b_2 C_{44} + b_3 C_{12} \quad . \tag{28}$$

The values of the a_i and b_i can be calculated from known values of the second order elastic constants and a knowledge of the propagation and polarization directions. Thus, the information obtained from a series of harmonic distortion experiments for a number of different propagation-polarization direction sets can be expressed as a set of linear equations

$$a_{1j} C_{111} + a_{2j} C_{112} + a_{3j} C_{144} + a_{4j} C_{166} + a_{5j} C_{123} + a_{6j} C_{456} = K_j \quad , \tag{29}$$

where j = 1, 2, 3 ... N and N is the number of experiments that have been performed. The right-hand side of Equation (29) is calculated from Equation (28) and is given by

$$K_j = \nu_j - b_{1j} C_{11} - b_{2j} C_{44} - b_{3j} C_{12} \quad , \tag{30}$$

where j = 1, 2, ... N.

The system of linear algebraic equations given by Equation (29) has the six third order elastic constants as unknowns. If Equation (29) includes six linearly independent equations then all six third order elastic constants can be found by means of the wave distortion experiments. The linear dependence or independence of Equations (29) is determined by the coefficients a_{ij} which may be calculated once the polarization and propagation directions are specified. Thus, a computer was used to try to find propagation-polarization direction sets yielding six linearly independent equations.

For values of the second order elastic constants corresponding to copper and also for values corresponding to gold, the best one could do was to find five linearly independent equations. In fact, for both copper and gold one finds that the relation

$$-2 a_{3j} + 4 a_{5j} + a_{6j} = 0 \tag{31}$$

holds for every obtainable equation. If Equation (31) is rewritten in the form

$$a_{3j} = 2 a_{5j} + \tfrac{1}{2} a_{6j} \tag{32}$$

and substituted into Equation (29), then the resulting system of equations is

$$a_{1j} C_{111} + a_{2j} C_{112} + a_{4j} C_{166} + (2 C_{144} + C_{123}) a_{5j} + (\tfrac{1}{2} C_{144} + C_{456}) a_{6j} = K_j \quad , \tag{33}$$

where $j = 1, 2, \ldots N$. The five quantities C_{111}, C_{112}, C_{166}, $(2 C_{144} + C_{123})$, and $(\frac{1}{2} C_{144} + C_{456})$ can, in principle, be determined by wave harmonic distortion experiments. The analytic argument given in the next sub-section shows that this result holds for any cubic material and for any measurement method for which the only strains used are single plane waves.

Proof of the Five Constant Result

The purpose of this sub-section is to show that the elastic constants C_{123}, C_{144}, and C_{456} can be replaced by the parameters $(2 C_{144} + C_{123})$ and $(\frac{1}{2} C_{144} + C_{456})$ in the expression for the elastic potential energy of a cubic crystal if only a single plane wave is present. Consider only that portion Ψ of the elastic potential energy expression Φ which contains C_{144}, C_{123}, and C_{456}; namely,

$$\bar{\Psi}(\bar{\eta}) = 2 C_{144} (\bar{\eta}_{11} \bar{\eta}_{23}^{2} + \bar{\eta}_{22} \bar{\eta}_{31}^{2} + \bar{\eta}_{33} \bar{\eta}_{12}^{2}) + C_{123} \bar{\eta}_{11} \bar{\eta}_{22} \bar{\eta}_{33} + 8 C_{456} \bar{\eta}_{12} \bar{\eta}_{23} \bar{\eta}_{31} \quad . \tag{34}$$

This expression is part of Equation (4) and here, as in the first part of the chapter, the bar over a quantity means it is measured with respect to the symmetry axes of the crystal. The coordinate system used for this

calculation is not along the symmetry axes, but is oriented so that the a_1 direction is along the direction of propagation. The change of coordinates in Ψ is accomplished by means of Equations (13) and (14). For convenience, Ψ is written in the form

$$\Psi(\eta) = f_1 C_{144} + f_2 C_{123} + f_3 C_{456} \quad , \tag{35}$$

where f_i is a function of η and R. If the equality

$$f_1 \equiv 2 f_2 + \frac{1}{2} f_3 \tag{36}$$

holds identically in η for each rotation matrix R, then the argument is complete since then C_{144}, C_{123}, and C_{456} appear in Ψ only as $(2 C_{144} + C_{123})$ and $(\frac{1}{2} C_{144} + C_{456})$.

To see that Equation (36) holds for each R, first notice that for a plane wave of arbitrary polarization the equation

$$J = \begin{pmatrix} 1 + \dfrac{\partial u_1}{\partial a_1} & 0 & 0 \\ \dfrac{\partial u_2}{\partial a_1} & 1 & 0 \\ \dfrac{\partial u_3}{\partial a_1} & 0 & 1 \end{pmatrix} \tag{37}$$

follows from Equations (18) and (5). Then, using Equation (1), the equality

$$\eta = \begin{pmatrix} \eta_{11} & \eta_{12} & \eta_{13} \\ \eta_{12} & 0 & 0 \\ \eta_{13} & 0 & 0 \end{pmatrix} \tag{38}$$

is obtained. However, one must exercise some caution before setting $\eta_{22} = \eta_{23} = \eta_{32} = \eta_{33} = 0$ in the expressions for f_1, f_2, and f_3 since the equations of motion, Equation (12), depend on $\frac{\partial \Phi}{\partial \eta_{ij}}$. It could be that some term in f_1 is zero without having a zero derivative. A closer inspection of Equation (12) shows that only $\frac{\partial \Phi}{\partial \eta_{1k}}$ appears; so a term containing η_{22}, η_{23}, η_{32}, or η_{33} as a factor will not contribute to the equations of motion. Substituting for f_i from Equation (34) yields the equation

$$2 f_2 + \tfrac{1}{2} f_3 - f_1 = 2 \bar{\eta}_{11}(\bar{\eta}_{22} \bar{\eta}_{33} - \bar{\eta}_{23}^2) + 2 \bar{\eta}_{31}(\bar{\eta}_{12} \bar{\eta}_{23} - \bar{\eta}_{22} \bar{\eta}_{31}) + 2 \bar{\eta}_{21}(\bar{\eta}_{32} \bar{\eta}_{13} - \bar{\eta}_{33} \bar{\eta}_{21}) \quad . \tag{39}$$

The right-hand side of Equation (39) is twice the value of det (η) which is invariant under rotations of the coordinate system. Since Equation (38) shows that det (η) = 0 in a particular coordinate system, one concludes that

$$2 f_2 + \tfrac{1}{2} f_3 - f_1 \equiv 0 \tag{40}$$

holds identically in η and R.

3. Tables of Useful Directions

The simplified form of the equations of motion, Equation (22) is of no use to the experimenter as it stands. This is because the coefficients μ and ν are such complicated functions of the polarization direction, the propagation direction, and second order elastic constants that choosing useful directions by means of hand calculations is out of the question. On the other hand, Equation (22) can be made useful for one who wishes to perform the experiments if the values of μ and expressions for ν are calculated by means of a computer and given as tables. In the first part of this section such tables are given for six cubic materials: copper, gold, sodium chloride, silicon, potassium chloride, and germanium. In the second part of the section the tables are used, along with preciously measured values of the elastic constants, to estimate the experimental uncertainties one could expect in the values of the elastic constants calculated from measured quantities.

Explanation of the Tables

Tables 1 through 6 represent the plane wave equations of motion for six different cubic materials. Each horizontal line of entries in the tables represents the equation of motion for a particular propagation direction and polarization direction. The entries in the table are given for a sufficiently large number of evenly spaced directions that interpolation between entires is possible. Thus, the tables can be used to obtain the continuous variation of μ and ν with propagation direction. The polarization and propagation directions are specified by unit vectors referred to the crystal symmetry axes rather than by Miller indices since the latter become cumbersome for such a large number of closely

spaced directions. In order to reduce the space required for the tables the irrelevant polarizations for which all of the coefficients of third order constants in Equation (29) are zero have been omitted. Because of the cubic symmetry only propagation directions whose unit vectors end on that portion of the surface of the unit sphere bounded by the spherical triangle with vertices at the points corresponding to the [100], [111], and [110] directions have been considered. Every other propagation direction is equivalent to one of these. It is interesting to note that propagation directions on the boundaries of this surface have only two relevant polarizations, i.e., polarizations for which the coefficients of at least one of the third order elastic constants in Equation (29) is nonzero, and that the [100] and [110] directions have only one relevant polarization each.

These tables have been prepared in order that one who wishes to do the experiments will have data which will assist him to choose optimum polarization and propagation directions for the determination of third order elastic constants. In making his selection, the experimentalist must also consider the variation of measurement error with polarization and propagation directions, the difficulties of cutting crystals for the various propagation directions, and the problem of exciting peculiar polarizations. Since these latter factors may vary among experimentalists, no attempt has been made to choose specific directions.

Estimated Uncertainties

Some rough calculations have been made to find out how the estimated maximum error for the experimentally measured values of ν_{jjj} would be reflected in the calculated maximum error for the values of the elastic

constants. To do this, several sets of 5 directions were chosen, each time using [100], [110], and [111] longitudinal polarizations with two additional polarizations in arbitrarily chosen directions. Then the value of ν for each direction was calculated from values of the elastic constants obtained by other methods (12). Finally, as if each ν had been measured with a maximum error of $\pm$ 5 per cent, the procedure was reversed and the numbers: C_{111}, C_{112}, C_{166}, $(2\ C_{144} + C_{123})$, and $(\frac{1}{2}\ C_{144} + C_{456})$ were calculated with their corresponding maximum errors. These calculations were done for two sets of directions each for copper and gold. The results in each case gave a maximum error for the values of C_{111}, C_{112}, and C_{166} on the order of 20 per cent. The calculated maximum errors for $(2\ C_{144} + C_{123})$ and $(\frac{1}{2}\ C_{144} + C_{456})$ were on the order of 1000 per cent. For the purpose of these calculations, the error introduced by the uncertainty in values of the second order elastic constants was neglected. One can conclude that C_{111}, C_{112}, and C_{166} can be measured with reasonable accuracy by the wave distortion technique, but that it may be difficult to measure $(2\ C_{144} + C_{123})$ and $(\frac{1}{2}\ C_{144} + C_{456})$ by this method.

4. Energy Flux Vector

In the preceding sections it has been assumed that the waves under consideration are infinite plane waves. An important geometrical consideration arises when one drops this assumption. Love (29), Waterman (30), and others (31) have pointed out that in an anisotropic solid a plane wave of finite extent will travel in the direction of the energy flux vector rather than the propagation direction. Figure 2 illustrates

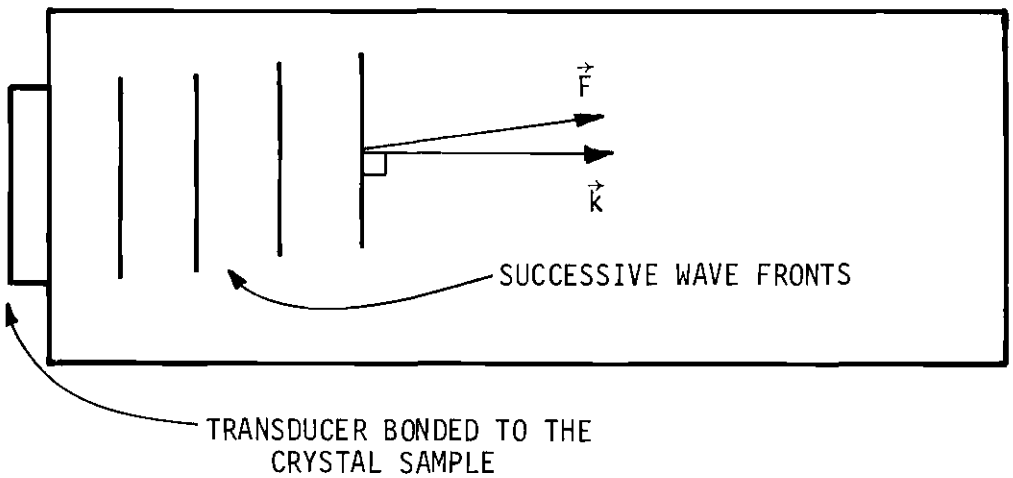


Figure 2. Deviation of the Energy Flux Vector from the Propagation Direction.

how a wave disturbance of finite extent can be a function of distance along the propagation direction, but travel in a quite different direction. This fact will affect the geometry of the wave distortion experiments because the largest wave generator one can devise is still of finite size and hence, in locating the generator and the detector on the sample, one would like to have the direction from the center of the generator to the center of the detector coincide with the direction of travel of the wave, which is the energy flux direction.

In this section the expression for the energy flux vector is derived by the method given in Love's book on elasticity (29). This expression is then applied to the case of a plane wave in a cubic crystal and finally, the energy flux direction is tabulated in a form which parallels that used in the tables for μ and ν in the preceding section of this chapter.

The elastic energy in a volume V of the continuum is given by the expression

$$E = \int_V \frac{1}{2} \rho \sum_{i=1}^{3} \dot{u}_i \dot{u}_i + \Phi \, dV_a \quad , \tag{41}$$

where ρ is the density per unit unstrained volume and u_i is defined by Equation (18). Since the deviation of the energy flux vector from the propagation direction is a consequence of the anisotropy of the continuum rather than a nonlinear effect, infinitesimal elasticity theory may be used here. The definition of the strain given in Equation (1) is shortened to

$$\eta_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial a_j} + \frac{\partial u_j}{\partial a_i} \right) , \tag{42}$$

and the cubic terms in the expression for Φ given by Equation (3) are dropped. To find an expression for the energy flux vector we would like to express the time rate of change of energy in V in terms of a surface integral over a surface bounding V. The integrand will then be identified as the energy flux vector into V. Since the positive sense of the surface normal vector is usually taken in the outward direction, the negative of the integrand will be taken as the actual expression for the energy flux vector across the surface.

The time rate of the change of the energy in V is given by

$$\frac{dE}{dt} = \int_V \rho \sum_{i=1}^{3} \dot{u}_i \ddot{u}_i + \sum_{i,j=1}^{3} \frac{\partial \Phi}{\partial \eta_{ij}} \frac{\partial \eta_{ij}}{\partial t} \, d^3a \quad , \tag{43}$$

where the infinitesimal definitions for η and Φ are used. As characteristic of the terms in Equation (43), take the terms containing $\dot{u}_1$ or $\frac{\partial \dot{u}_1}{\partial a_j}$ as a factor. These can be simplified by integration by parts to give

$$\int_V \rho \, \dot{u}_1 \ddot{u}_1 + \sum_{j=1}^{3} \frac{\partial \Phi}{\partial \eta_{1j}} \frac{\partial \dot{u}_1}{\partial a_j} \, dV_a = \int_V \dot{u}_1 \left\{ \rho \, \ddot{u}_1 - \sum_{j=1}^{3} \frac{\partial}{\partial a_j} \frac{\partial \Phi}{\partial \eta_{1j}} \right\} \tag{44}$$

$$+ \sum_j \frac{\partial}{\partial a_j} \left(\dot{u}_1 \frac{\partial \Phi}{\partial \eta_{1j}} \right) dV_a \quad .$$

The term given in the brackets vanishes identically because of the equation of motion for infinitesimal elasticity theory. Equation (43) can be

rewritten

$$\frac{dE}{dt} = \int_V \sum_{i,j=1}^{3} \frac{\partial}{\partial a_j} \left(\dot{u}_i \frac{\partial \Phi}{\partial \dot{\eta}_{ij}} \right) dV_a = \int_S \sum_{i,j=1}^{3} \dot{u}_i \frac{\partial \Phi}{\partial \dot{\eta}_{ij}} \, dS_j \quad , \tag{45}$$

so that the energy flux vector is given by

$$F_j = - \sum_{i=1}^{3} \dot{u}_i \frac{\partial \Phi}{\partial \dot{\eta}_{ij}} \quad . \tag{46}$$

In the case of plane waves the expression for u_i is

$$u_i(a_i,t) = A\hat{P}_i \sin \left(\omega t - \sum_{j=1}^{3} k_j a_j \right) \quad , \tag{47}$$

where A is the amplitude of the plane wave, $\hat{P}_i$ is the polarization unit vector of the plane wave, ω is the angular frequency, and k_j is the propagation vector. Differentiating Equation (47) yields

$$\dot{u}_i = A\hat{P}_i \, \omega \cos \left(\omega t - \sum_{j=1}^{3} k_j a_j \right) \quad , \tag{48}$$

which can be used along with the derivative of the expression for Φ,

$$\frac{\partial \Phi}{\partial \dot{\eta}_{ij}} = \sum_{k,\ell=1}^{3} C_{ijk\ell} \dot{\eta}_{k\ell} \quad , \tag{49}$$

to obtain the expression

$$F_j = - \sum_{ik\ell=1}^{3} A^2 \omega C_{ijk\ell} \hat{P}_i \hat{P}_k k_\ell \cos^2 \left(\omega t - \sum_{m=1}^{3} k_m a_m \right) \quad , \tag{50}$$

which is the energy flux vector for plane waves in a crystal. By averaging over one period and using the symmetry properties for a cubic crystal, one obtains

$$\langle F_1 \rangle = \frac{A^2 \omega}{2} \left\{ \frac{C_{11}}{2} \hat{P}_1^2 k_1 + \frac{C_{44}}{2} (\hat{P}_2 \hat{P}_1 k_2 + \hat{P}_2 \hat{P}_2 k_1) \right. \tag{51}$$

$$\left. + \frac{C_{44}}{2} (\hat{P}_3 \hat{P}_1 k_3 + \hat{P}_3 \hat{P}_3 k_1) + \frac{1}{2} C_{12} (\hat{P}_1 \hat{P}_2 k_2 + \hat{P}_1 \hat{P}_3 k_3) \right\} ,$$

$$\langle F_2 \rangle = \frac{A^2 \omega}{2} \left\{ \frac{C_{11}}{2} \hat{P}_2^2 k_2 + \frac{C_{44}}{2} (\hat{P}_1 \hat{P}_2 k_1 + \hat{P}_1 \hat{P}_1 k_2) \right.$$

$$\left. + \frac{C_{44}}{2} (\hat{P}_3 \hat{P}_2 k_3 + \hat{P}_3 \hat{P}_3 k_2) + \frac{C_{12}}{2} (\hat{P}_2 \hat{P}_1 k_1 + \hat{P}_2 \hat{P}_3 k_3) \right\} ,$$

and

$$\langle F_3 \rangle = \frac{A^2 \omega}{2} \left\{ \frac{C_{11}}{2} \hat{P}_3^2 k_3 + \frac{C_{44}}{2} (\hat{P}_1 \hat{P}_3 k_1 + \hat{P}_1 \hat{P}_1 k_3) \right.$$

$$\left. + \frac{C_{44}}{2} (\hat{P}_2 \hat{P}_3 k_2 + \hat{P}_2 \hat{P}_2 k_3) + \frac{C_{12}}{2} (\hat{P}_3 \hat{P}_2 k_2 + \hat{P}_3 \hat{P}_1 k_1) \right\} .$$

These expressions have been normalized and programmed for a computer to obtain Tables 6 to 12. Here, the format of Tables 1 through 6 has been retained so that when one chooses a propagation and polarization direction set from the first group of tables he may then refer to the second set to see how the energy flux vector will affect the geometry of the experiment. The importance of this effect is demonstrated by the fact that some of the tabulated deviations are as large as 20 degrees.

5. Summary and Concluding Remarks

The purpose of this chapter was to describe the research which led to the solution of some theoretical problems involved in measuring third

order elastic constants of cubic crystals by the wave harmonic distortion method. In particular, four problems were considered, namely, to simplify the equations of motion, to find out how many elastic constants can be measured, to show how to choose useful directions, and to show how the geometry of the experiment is affected by the deviation of the energy flux vector from the propagation direction.

The first of these problems was discussed in the first section of the chapter, where it was shown that for a linearly polarized plane wave of a suitably chosen polarization direction the equation of motion can be written in the form

$$\rho P_{tt} = \mu P_{aa} + \nu P_a P_{aa} \quad ,$$

where P is the displacement in the polarization direction, a is distance along the propagation direction, ρ is the density, μ is a linear combination of second order elastic constants, and ν is a linear combination of second and third order elastic constants. A perturbation solution of this equation was written out and it was pointed out that the quantity ν could be calculated from the results of a wave harmonic distortion experiment.

The research described in the second section of the chapter shows that the parameters C_{111}, C_{112}, C_{166}, $(2 C_{144} + C_{123})$, and $(\frac{1}{2} C_{144} + C_{456})$ can, in principle, be measured by means of these experiments. This result was obtained with the help of a computer and is substantiated by an algebraic argument. A calculation made in the third section of the chapter indicates that there may be some practical difficulties in measuring the last two of these parameters by this method.

Useful directions for measuring linear combinations of third order elastic constants can be found with the help of the tables given in the third section of this chapter. These tables have been made for six particular materials and provide sufficient information for interpreting the results of the experiments.

Finally, the geometry problem was solved in the fourth section by means of tables which give the proper relative position of the ultrasonic generator and detector on the crystal sample. The ultrasonic wave actually travels in the direction of the energy flux vector rather than the propagation direction so that one would like to have the direction from the center of the generator to the center of the detector coincide with the energy flux direction for the propagation direction chosen. The tables give the energy flux direction for each of the useful directions given in the preceding section.

In conclusion, it should be mentioned that although the wave harmonic distortion method cannot be used by itself to measure a complete set of elastic constants, it can be used in conjunction with another technique to measure a complete set. Linear combinations of elastic constants can be calculated from the results of experiments measuring the change in sound velocity in the crystal due to an applied uniaxial or hydrostatic strain (8). Unfortunately, an applied uniaxial strain is apt to cause slip or plastic deformation in soft crystals such as copper (9), and the sound velocity measurements for the case of hydrostatic pressure do not yield enough information to measure a complete set of constants. However, a complete set of elastic constants for a cubic crystal can be obtained by combining the results of hydrostatic pressure

sound velocity experiment with results of wave harmonic distortion experiments (17). Both of these techniques are well suited for soft crystals, and recently Gauster (14) has published a complete set of third order elastic constants for copper which was calculated this way.

CHAPTER III

BEAM SCATTERING EXPERIMENTS

Several authors (21-23) have suggested that measurements of third order elastic constants might be accomplished by means of ultrasonic beam scattering experiments. Such measurements would utilize the fact that the production of a scattered wave by the interaction of two non-collinear ultrasonic beams is due to the elastic nonlinearities of the solid. The most obvious method for utilizing this fact is to measure the amplitudes of the input and scattered waves and to use these amplitudes to calculate a linear combination of the third order elastic constants. To do this, one needs to know how the amplitudes of the three waves are related to the elastic constants.

The first section of this chapter is devoted to the derivation of an equation relating the wave amplitudes to the elastic constants of the solid. For this derivation the displacement field is quantized and the interaction of the ultrasonic beams is represented by the interaction of the quanta of the corresponding phonon branches. The long wave length approximation is used; that is, dispersion has been neglected. Time dependent perturbation theory is used to obtain the final result.

In the second section of the chapter the theory is applied to the case of cubic materials in order to determine, out of the totality of interactions which occur between two incident beams, which interactions are experimentally useful for determining third order elastic constants.

Specific interactions are suggested for six materials and a sample calculation is made in order to demonstrate how one can use the measured quantities for these interactions to calculate third order elastic constants.

Some suggestions for doing the experiment are given along with the concluding remarks in the final section of the chapter.

1. Theory of Three Phonon Interactions

In this section the classical Hamiltonian for the continuum is quantized and first order time dependent perturbation theory is used to derive an expression for the density of scattered phonons in terms of the input phonon densities and the third order elastic constants (1). Since the phonon densities can then be related to the wave amplitudes (23), the result is an equation which relates the elastic constants to quantities which can be measured.

In this derivation the quantum, rather than classical, formalism is used because it allows some algebraic shortcuts. Taylor and Rollins (23) have shown that for isotropic solids the quantum and classical predictions are identical and one would expect the same result here.

The classical Hamiltonian for a perfectly elastic continuum is given by the expression

$$H = \frac{1}{2} \int_V \left[\rho^{-1} \sum_{b=1}^{3} p_b \, p_b \right] dV + \int_V \Phi(\eta) \, dV \quad , \tag{52}$$

where the momentum density, p_k, is given by $p_k = \rho \dot{u}_k$, the expression for $\Phi(\eta)$ is given in Equation (3), V is the interaction volume, and u_k is defined by Equation (18). The surface energy term, which couples the

interaction volume with the rest of the solid, has been omitted here because one would expect it to be much smaller than the terms retained. The symmetric strain tensor is defined in Equation (1) which, for this derivation, is rewritten as

$$\eta_{jk} = \frac{1}{2}\left(\sum_{b=1}^{3} u_{b;j}\, u_{b,k} + u_{j,k} + u_{k,j} \right) \tag{53}$$

by means of Equation (18). In this equation and in the expressions that follow, the subscripts j and k take on the values 1, 2, and 3 and the symbol $u_{b,j}$ is defined by the equation

$$u_{b,j} = \frac{\partial u_b}{\partial a_j} \quad .$$

Equations (53) and (3) can be substituted into Equation (52) to obtain the Hamiltonian in the form

$$H = H_o + H' \quad , \tag{54}$$

where H_o and H' are given by the expressions

$$H_o = \frac{1}{2} \int_V \left[\sum_{b=1}^{3} \rho^{-1} p_b\, p_b \right] dV + \frac{1}{2!} \int_V \left[\sum_{\substack{b,c \\ d,e}} C_{bcde}\, u_{b,c}\, u_{d,e} \right] dV \tag{55}$$

and

$$H' = \int_V \left\{ \frac{1}{2!} \sum_{bcdef} C_{bcde}\, u_{b,c}\, u_{f,d}\, u_{f,e} + \frac{1}{3!} \sum_{bcdefg} C_{bcdefg}\, u_{b,c}\, u_{d,e}\, u_{f,g} \right\} dV \, . \tag{56}$$

In writing these expressions, use is made of the following symmetry properties of C_{bcde} and C_{bcdefg} which are common to all materials:

$$C_{bcde} = C_{debc} = C_{ed\ bc} = \text{etc.} \quad , \tag{57}$$

and

$$C_{bcdefg} = C_{de\ bc\ fg} = C_{ed\ bcfg} = \text{etc.}$$

As in the preceding chapter, all terms in the elastic energy containing powers of $u_{j,k}$ greater than the third have been dropped since their effect is negligible for the range of the parameters one can realize in current experiments. Equations (54-56) are exact up to this point.

Quantization of H_o

In the quantum theory, the variables u_j and p_j in Equation (55) are canonically conjugate operators which obey the commutation relation

$$[u_k(\vec{a}),\ p_j(\vec{a}')] = i\hbar\, \delta(\vec{a} - \vec{a}')\, \delta_{kj} \quad . \tag{58}$$

In this equation, $\delta(\vec{a} - \vec{a}')$ is the Dirac delta function, δ_{kj} is the Kronecker δ, and $\hbar$ is the normalized Planck's constant.

In order to use existing perturbation theories, one needs to write the Hamiltonian in terms of the raising and lowering operators. These raising and lowering operators form discrete sets, while the operators $u_k(\vec{a})$ and $p_k(\vec{a})$ in Equation (58) are functions of the continuously varying quantity, $\vec{a}$. Consequently, $u_k(\vec{a})$ and $p_k(\vec{a})$ are transformed according to the equations

$$u_j(\vec{a}) = \frac{1}{\sqrt{V}} \sum_{\vec{q}} U^j_{\vec{q}}\, e^{i\vec{q} \cdot \vec{a}} \tag{59}$$

and

$$p_j(\vec{a}) = \frac{1}{\sqrt{V}} \sum_{\vec{q}} P^j_{\vec{q}}\, e^{-i\vec{q} \cdot \vec{a}} \quad . \tag{60}$$

In these expressions the symbol $\sum_{\vec{q}}$ represents a discrete sum over the normal mode frequencies of the interaction volume and $\vec{q}$ is the propagation vector corresponding to a given frequency. By substituting Equation (59) and Equation (60) into Equation (55) and using the identity

$$\frac{1}{V} \int e^{i(\vec{q} - \vec{q}')} \cdot \vec{a}\, dV = \delta_{\vec{q}\,\vec{q}'} \quad , \tag{61}$$

one obtains

$$H_o = \sum_{\vec{q}} \sum_{b=1}^{3} (2\rho)^{-1} P^b_{\vec{q}}\, P^{b*}_{\vec{q}} \tag{62}$$

$$+ \frac{1}{2!} \sum_{\vec{q}} \sum_{bcde} C_{bcde}\, U^b_{\vec{q}}\, U^{d*}_{\vec{q}}\, q_c\, q_e \quad ,$$

where P^* is the Hermitian conjugate of P. In writing H_o in this form the identities

$$U^{k*}_{\vec{q}} = U^k_{-\vec{q}} \quad \text{and} \quad P^k_{\vec{q}} = P^{k*}_{-\vec{q}} \tag{63}$$

have been used. These identities follow from the Hermitian property of the operators u_j and p_k.

For each $\vec{q}$, Equation (62) is the Hamiltonian of a system of quantized coupled linear oscillators. In order to express this Hamiltonian in terms of raising and lowering operators, it is first necessary to write it in terms of the normal coordinates for each $\vec{q}$. The symmetry properties given by Equation (57) guarantee that the matrix

$$W^{\vec{q}}_{jk} = \frac{1}{2} \sum_{b,c=1}^{3} C_{jbkc}\, q_b\, q_c \tag{64}$$

will be symmetric, and so for each $\vec{q}$ there exists an orthogonal matrix, call it $R^{\vec{q}}$, such that

$$\frac{1}{2} \sum_{bcde} R^{\vec{q}}_{kb}\, R^{\vec{q}}_{jd}\, C_{bcde}\, q_c\, q_e = M^{\vec{q}}_{k}\, \delta_{jk} \quad . \tag{65}$$

The symbol $M^{\vec{q}}_{k}$ represents the eigenvalues of the matrix $W^{\vec{q}}_{jk}$. The transformation to normal coordinates can be accomplished by substituting

$$U^{k}_{\vec{q}} = \sum_{b=1}^{3} R^{\vec{q}}_{bk}\, V^{\vec{q}}_{b} \tag{66}$$

and

$$P^{k}_{\vec{q}} = \sum_{b=1}^{3} R^{\vec{q}}_{bk}\, \Pi^{\vec{q}}_{b} \tag{67}$$

into Equation (62). The result of this transformation is

$$H_o = \sum_{\vec{q}} \left\{ \frac{1}{2\rho} \sum_{b=1}^{3} \Pi^{\vec{q}}_{b}\, \Pi^{\vec{q}\,*}_{b} + \sum_{b=1}^{3} M^{\vec{q}}_{b}\, V^{\vec{q}}_{b}\, V^{\vec{q}\,*}_{b} \right\} \quad . \tag{68}$$

The raising and lowering operators are defined by the equations

$$a_k^{\vec{q}} = \left(2\hbar \rho \omega_k^{\vec{q}} \right)^{-\frac{1}{2}} \Pi_k^{\vec{q}} - i \left(\rho \omega_k^{\vec{q}} / 2\hbar \right)^{\frac{1}{2}} V_k^{\vec{q}*} \tag{69}$$

and

$$a_k^{\vec{q}*} = \left(2\hbar \rho \omega_k^{\vec{q}} \right)^{-\frac{1}{2}} \Pi_k^{\vec{q}*} + i \left(\rho \omega_k^{\vec{q}} / 2\hbar \right)^{\frac{1}{2}} V_k^{\vec{q}} \quad , \tag{70}$$

where $\omega_k^{\vec{q}} = \sqrt{2 M_k^{\vec{q}} / \rho}$ and $i^2 = -1$. The commutation relations for $a_k^{\vec{q}}$ and $a_k^{\vec{q}*}$ are given by the expression

$$\left[a_j^{\vec{q}} , a_k^{\vec{q}'*} \right] = \delta_{\vec{q}\,\vec{q}'} \delta_{jk} \quad , \tag{71}$$

which can be deduced from Equation (58) by means of the equations defining the transformations just accomplished on H_o. The linear part of the Hamiltonian may now be written

$$H_o = \hbar \sum_{\vec{q}} \sum_{b=1}^{3} \left\{ \frac{1}{2} + a_b^{\vec{q}*} a_b^{\vec{q}} \right\} \omega_b^{\vec{q}} \quad . \tag{72}$$

If the symbol $| \ldots N_k^{\vec{q}} \ldots \rangle$ represents an eigenvector of H_o for which the occupation number (eigenvalue) corresponding to the mode defined by $(\vec{q},k)$ is $N_k^{\vec{q}}$ then the nonzero matrix elements of $a_k^{\vec{q}}$ and $a_k^{\vec{q}*}$ are given by the equations

$$\langle \ldots N_k^{\vec{q}} - 1 \ldots | a_k^{\vec{q}} | \ldots N_k^{\vec{q}} \ldots \rangle = \sqrt{N_k^{\vec{q}}} \tag{73}$$

and

$$\left\langle \ldots N_k^{\vec{q}} + 1 \ldots \mid a_k^{\vec{q}*} \mid \ldots N_k^{\vec{q}} \ldots \right\rangle = \sqrt{N_k^{\vec{q}} + 1} \quad . \tag{74}$$

Transition Probability due to H′

The transformations defined in the preceding paragraphs can now be used to calculate the matrix elements, and thence the transition probability, from the nonlinear part of the Hamiltonian. By performing the three transformations defined by Equations (59) and (60), Equations (66) and (67), and Equations (69) and (70) on the expression for H′ given in Equation (56), one obtains

$$H' = \frac{(2\hbar)^{3/2}}{8\rho^{3/2}\sqrt{V}} \sum_{\substack{\vec{q}\vec{q}'\vec{q}'' \\ bcd}} \left\{ \left(\frac{1}{2!} \sum_{\substack{ef \\ gh\ell}} C_{efgh} R_{bg}^{\vec{q}} R_{c\ell}^{\vec{q}'} R_{d\ell}^{\vec{q}''} q_h q_e' q_f'' \right. \right. \tag{75}$$

$$\left. + \frac{1}{3!} \sum_{\substack{rst \\ uvw}} C_{rstuvw} R_{br}^{\vec{q}} R_{ct}^{\vec{q}'} R_{dv}^{\vec{q}''} q_s q_u' q_w'' \right)$$

$$\cdot \left(a_b^{\vec{q}} - a_b^{\vec{q}*} \right) \left(a_c^{\vec{q}'} - a_c^{\vec{q}'*} \right) \left(a_d^{\vec{q}''} - a_d^{\vec{q}''*} \right) \left(\omega_b^{\vec{q}} \omega_c^{\vec{q}'} \omega_d^{\vec{q}''} \right)^{-\frac{1}{2}}$$

$$\left. \cdot \delta_{o,\, \vec{q} + \vec{q}' + \vec{q}''} \right\} \quad ,$$

where $\delta_{o,\, \vec{q} + \vec{q}' + \vec{q}''}$ expresses the momentum conservation requirement. The clutter of subscripts and superscripts in Equation (75) can be cleaned up if one notices that the elements of the set $(\vec{q},k)$, which are the superscript and subscript of the operator $a_k^{\vec{q}}$, designate a phonon state in the following way: The vector $\vec{q}$ is the propagation vector of the phonon. Its direction is the direction of propagation and

its magnitude is $2\pi/\lambda$, where λ is the wavelength. The integer k defines the polarization direction of the phonon state, that is, the phonon state $(\vec{q},k)$ is polarized along the unit vector

$$\hat{P}_j = R^{\vec{q}}_{kj} \quad , \tag{76}$$

which is defined in Equation (65). In the physical situation to be described here there are ideally only three occupied phonon states, namely, the two scattering states and the scattered state. If these states are called 1, 2, and 3, then the set $(\vec{q},k)$ can be replaced by the integer j. The symbol $\hat{P}^k_j$ will then be used in place of the symbol $R^{\vec{q}}_{kj}$ to represent the polarization unit vector. That is, $\hat{P}^k_j$ will be the jth coordinate of the polarization vector of state k. Similarly, q^k_j will be the jth coordinate of the propagation vector of the state k.

To further simplify Equation (75), one can anticipate the energy conservation requirement of time dependent perturbation theory by dropping those terms of the sum which cannot conserve energy. In particular, three phonons cannot be simultaneously annihilated or created. Also, if state 3, the scattered phonon state, is regarded as initially unpopulated, then an event annihilating a phonon in this state is prohibited. This leaves two possibilities: annihilation of both scattering phonons accompanied by creation of a scattered phonon or annihilation of one scattering phonon accompanied by creation of a scattered phonon and creation of a phonon in the other scattering state. These two possibilities are represented by the rewritten expressions for H′,

$$H' = \frac{(2\hbar)^{3/2}}{8(\rho)^{3/2}\sqrt{V}} \cdot G.(q^1\ q^2\ q^3).(\omega_1\ \omega_2\ \omega_3)^{-\frac{1}{2}} \cdot a^1\ a^2\ a^{3*} \tag{77}$$

and

$$H' = \frac{(2\hbar)^{3/2}}{8\rho^{3/2}\, V^{\frac{1}{2}}} \cdot G \cdot (q^1\, q^2\, q^3) \cdot (\omega_1\, \omega_2\, \omega_3)^{-\frac{1}{2}}\, a^1\, a^{2*}\, a^{3*} \quad , \quad (78)$$

where Equation(77) applies if $\vec{q}^1 + \vec{q}^2 = \vec{q}^3$, and Equation (78) applies if $\vec{q}^1 - \vec{q}^2 = \vec{q}^3$. The factor G is given by the expression

$$G = \frac{1}{2!} \sum_{efgh\ell} 2\, C_{efgh} \left(\hat{P}^1_g\, \hat{P}^2_\ell\, \hat{P}^3_\ell\, \hat{q}^1_h\, \hat{q}^2_e\, \hat{q}^3_f \right. \quad (79)$$

$$\left. + \hat{P}^2_g\, \hat{P}^3_\ell\, \hat{P}^1_\ell\, \hat{q}^2_h\, \hat{q}^3_e\, \hat{q}^1_f + \hat{P}^3_g\, \hat{P}^1_\ell\, \hat{P}^2_\ell\, \hat{q}^3_h\, \hat{q}^1_e\, \hat{q}^2_f \right)$$

$$+ \frac{1}{3!} \sum_{rstuvw} 6\, C_{rstuvw}\, \hat{P}^1_r\, \hat{P}^2_t\, \hat{P}^3_v\, \hat{q}^1_s\, \hat{q}^2_u\, \hat{q}^3_w \quad .$$

In these equations q^k is the magnitude of the propagation vector of the kth state and $\hat{q}^k_j$ is the unit vector in the propagation direction.

Let the symbol $| N_1, N_2, 0 \rangle$ represent the initial state of the system. If the perturbing Hamiltonian is given by Equation (77) then, by using Equations (73) and (74) one can see that the only possible transition will be to the state $| N_1 - 1, N_2 - 1, 1 \rangle$. If the perturbing Hamiltonian is that of Equation (78) then the final state will be $| N_1 - 1, N_2 + 1, 1 \rangle$. If H'_{if} represents the matrix element of the perturbing Hamiltonian between the final and initial states then

$$H'_{if} = \frac{(2\hbar)^{3/2}\, G\, q^1\, q^2\, q^3\, (\omega_1\, \omega_2\, \omega_3)^{-\frac{1}{2}}}{8\rho^{3/2}\, V^{\frac{1}{2}}} \sqrt{N_1\, N_2} \quad (80)$$

and

$$H'_{if} = \frac{(2\hbar)^{3/2}\, G\, q^1\, q^2\, q^3\, (\omega_1\, \omega_2\, \omega_3)^{-\frac{1}{2}}}{8\rho^{3/2}\, V^{\frac{1}{2}}} \sqrt{N_1\, (N_2 + 1)} \quad , \qquad (81)$$

where Equation (80) follows from Equation (77) and Equation (81) follows from Equation (78). In the calculations that follow, it is assumed that $N_2 \gg 1$ so that Equations (80) and (81) can be regarded as identical.

The transition probability predicted by first order time dependent perturbation theory is given by

$$P = \frac{2\pi}{\hbar} (H'_{if})^2 \mathcal{D}_f \quad , \qquad (82)$$

where P represents the number of occurrences per second and the density of final states, $\mathcal{D}_f$, is given by

$$\mathcal{D}_f = \frac{V(\omega_3)^2}{2\hbar\, \pi^2 (C_3)^3} \quad . \qquad (83)$$

In this expression, C_3 is the phase velocity of a phonon in state 3. Substituting Equation (83) and Equation (80) into Equation (82) one obtains the expression

$$P = \frac{2\hbar\, G^2\, N_1\, N_2 (\omega_3)^2\, (q^1\, q^2\, q^3)^2}{16\, \pi\, \rho^3 (\omega_1\, \omega_2\, \omega_3)\, (C_3)^3} \quad , \qquad (84)$$

which is the number of state 3 phonons per second created at the intersection of the beams. This expression can be rewritten by means of the identity $C_k = \frac{\omega_k}{q^k}$ to give

$$P = \frac{2\hbar\, G^2\, N_1\, N_2\, \omega_1\, \omega_2 (\omega_3)^3}{(C_1\, C_2)^2\, (C_3)^5} \quad . \qquad (85)$$

Scattered Wave Amplitude

Two things remain to be done in order to obtain an expression for predicting the scattered wave amplitudes. First, the transition probability, P, must be used to find the state 3 phonon density in the scattered beam and second, the phonon density needs to be related to the amplitude of a classical wave.

Regard the scattered wave as a phonon beam having cross-sectional area S. Then, since P phonons of state 3 are created each second at the interaction volume, one must observe P state 3 phonons per second crossing a plane in the scattered beam. In other words,

$$P = n_3 C_3 S \quad , \tag{86}$$

where n_3 is the phonon density in the scattered beam. Rewriting Equation (86) to give n_3 and substituting from Equation (85) yields

$$n_3 = \frac{2\hbar G^2 N_1 N_2 \omega_1 \omega_2 (\omega_3)^3}{S(C_1 C_2)^2 (C_3)^6} \quad . \tag{87}$$

The phonon density, n_k, in a beam of coherent phonons can be related to the classical wave amplitude by means of an argument due to Taylor and Rollins. Briefly, the classical and quantum expressions for the energy flux across a plane of constant phase are equated and the resulting identity is solved for the classical wave amplitude.

The classical energy flux vector given in Equation (50) can be averaged over one period to give

$$F_j^k = -\tfrac{1}{2} \sum_{bcd} A_k^2 \omega_k C_{bjcd} \hat{P}_b^k \hat{P}_c^k q_d^k \quad . \tag{88}$$

The component of this vector perpendicular to a plane of constant phase is given by the expression

$$I_k = \sum_e \frac{1}{q^k} F_e^k q_e^k = \frac{A_k^2 \omega_k}{2q^k} \sum_{bcde} C_{becd} \hat{P}_b^k \hat{P}_c^k q_e^k q_j^k \quad . \tag{89}$$

This can be simplified by means of Equation (64) and the definition of ω_k given in Equation (70) to give

$$I_k = \frac{A_k^2 \omega_k}{q^k} \frac{(\omega_k)^2 \rho}{2} \quad . \tag{90}$$

Finally, the substitution $C_k = \frac{\omega_k}{q^k}$ yields

$$I_k = \frac{A_k^2}{2} \rho C_k (\omega_k)^2 \quad . \tag{91}$$

The corresponding quantum mechanical expression is

$$I_k = n_k \hbar \omega_k C_k \quad . \tag{92}$$

By equating the right-hand sides of Equations (90) and (91) and solving for the classical wave amplitude, A_k, one obtains

$$A_k = \sqrt{\frac{2n_k \hbar}{\rho \omega_k}} \quad , \tag{93}$$

and conversely,

$$n_k = \frac{N_k}{V} = \frac{A_k^2 \rho \omega_k}{2\hbar} \quad . \tag{94}$$

The final expression for the amplitude of the scattered wave is obtained by substituting Equations (93) and (94) into Equation (87) to give

$$A_3 = \frac{G\, V\, A_1\, A_2\, \omega_1\, \omega_2\, \omega_3}{\rho\, c_1\, c_2\, (c_3)^3\, (16\, \pi\, S)^{\frac{1}{2}}} \quad . \tag{95}$$

Except for the factor $(16\, \pi\, S)^{-\frac{1}{2}}$, this final expression agrees with the analogous expression obtained by Taylor and Rollins (23) for isotropic solids. The discrepancy occurs because of a difference in the means used for describing the geometry of the scattered wave. Thus, if one measures A_1, A_2 and A_3 for a particular interaction along with the geometrical parameters of the experiment, V and S, then Equation (95) can be used to calculate a value for a linear combination of elastic constants given by G. Hopefully, enough of these linear combinations could be measured to allow one to calculate a complete set of third order elastic constants.

The purpose of this section of the chapter was to derive an equation relating elastic constants to quantities that can be measured experimentally. Equation (95) is such an equation provided that one knows the quantity G for the interaction he happens to be using. In the next section some potentially useful interactions for cubic materials are listed, along with corresponding expressions for G, so that Equation (95) is rendered useful for one who wishes to do the experiment.

2. Calculations

The calculations presented here are based on the theoretical results obtained in the preceding section and have as their goal the prediction of interaction sets for cubic materials which would be useful

for measuring third order elastic constants. The problem can be divided into two parts. First, one needs to find which interactions are allowed, and second, one needs to select useful interactions from the set of allowed interactions.

Finding Allowed Interactions

The equation for the amplitude of a scattered wave, Equation (95), is valid only for the case of resonant scattering, that is, scattering for which the interaction parameters satisfy the conservation laws for energy and momentum. These laws are given by the equations

$$\omega_1 \pm \omega_2 = \omega_3 \tag{96}$$

and

$$\vec{q}^1 \pm \vec{q}^2 = \vec{q}^3 \quad , \tag{97}$$

where the choice of + or - depends on whether the interaction is of the type given in Equation (77) or of the type given in Equation (78).

The problem of finding allowed interactions can be reduced to finding a solution to a set of algebraic equations. By means of the identity $q^k = \frac{\omega_k}{C_k}$, which holds because dispersion is negligible at the frequencies being considered, Equations (96) and (97) can be rewritten in the form

$$1 + \frac{\omega_2}{\omega_1} = \frac{\omega_3}{\omega_1} \quad , \tag{98}$$

$$\frac{1}{C_1} \hat{q}_k^1 + \frac{\omega_2}{\omega_1} \cdot \frac{1}{C_2} \cdot \hat{q}_k^2 = \frac{\omega_3}{\omega_1} \frac{1}{C_3} \hat{q}_k^3 \quad ,$$

where $\hat{q}_k^j$ is the kth component of the normalized propagation vector for state j. In this equation one allows $\frac{\omega_2}{\omega_1}$ and $\frac{\omega_3}{\omega_1}$ to be positive or negative, thus eliminating the need for the ± sign used in Equations (96) and (97). The input polarization and propagation directions are now regarded as given, so that the problem of finding a resonant interaction is equivalent to finding a unit vector $\hat{q}_k^3$ and two scalars, $\frac{\omega_2}{\omega_1}$ and $\frac{\omega_3}{\omega_1}$, such that Equation (98) is satisfied. Let the set of unknowns $\hat{q}_k^3$, $\frac{\omega_2}{\omega_1}$, and $\frac{\omega_3}{\omega_1}$ be represented by χ_b, b = 1, 2, ... 5. Then Equation (98) can be written in the form

$$D_k + E_k \chi_4 - F \chi_5 \chi_k = 0 \qquad (99)$$

$$1 + \chi_4 - \chi_5 = 0$$

$$\chi_1^2 + \chi_2^2 + \chi_3^2 - 1 = 0 \quad ,$$

where $D_k = \frac{1}{C_1} \hat{q}_k^1$ and $E_k = \frac{1}{C_2} \hat{q}_k^2$ are fixed by the choice of input waves, and $F = \frac{1}{C_3}$ is a function of χ_1, χ_2, χ_3, and an integer, j, which designates the choice of the scattered wave polarization.

Notice that Equation (99) illustrates a difficulty involved in finding allowed interactions in anisotropic solids. For the case of isotropic solids the quantity F depends only on j, the polarization of the scattered wave. Studies of three phonon interactions in isotropic solids have produced complicated selection rules which specify combinations of scattering and scattered wave polarizations lead to a solution of Equation (99). On the other hand, in an anisotropic solid the quantity F depends on the solution of a cubic equation, the eigenvalue problem of

Equation (64), and so the problem of finding selection rules is hopelessly complicated. Because of these complications, no attempt has been made here to formulate a set of general selection rules. Instead, specific allowed interactions for cubic crystals have been found by means of a method of successive approximations and the suggested useful interactions were chosen from these.

The computer program used to find these allowed interactions uses the following calculational procedure. As in the discussion above, the scattering polarization and propagation directions are fixed inputs and the quantities $\hat{q}_k^3$, $\frac{\omega_2}{\omega_1}$, and $\frac{\omega_3}{\omega_1}$ are the unknowns. To begin, a value is assumed for the quantity $\frac{\omega_2}{\omega_1}$. This determines a trial value for the vector $\frac{\omega_3}{\omega_1}\frac{1}{C_3}\hat{q}_k^3$ by means of the second equation of Equation (98). By normalizing this vector and choosing a particular scattered wave polarization the quantity C_3 can be obtained and consequently, $\frac{\omega_3}{\omega_1}$. Finally, the quantity

$$1 + \frac{\omega_2}{\omega_1} - \frac{\omega_3}{\omega_1} = \Omega_3 \tag{100}$$

is calculated. If Ω_3 were zero then the conservation laws would be satisfied. To that end, the value of $\frac{\omega_2}{\omega_1}$ is varied in successive iterations until $/\Omega_3/$ is less than some given tolerance. Finally, it should be mentioned that, although this method has been very successful in calculating allowed interactions, there is no guarantee that the method will converge for every allowed interaction.

Useful Interactions

The reason for finding resonant interactions between ultrasonic

beams in an anisotropic solid is to suggest some specific interactions which might be useful for measuring third order elastic constants. Because of the difficulties involved in exciting unusual polarization modes, a particular interaction is more likely to be useful if the directions involved are directions for which "pure mode" propagation exists. By "pure mode" propagation one means that the uncoupled polarization direction is either parallel to or perpendicular to the propagation direction. For cubic crystals the principal propagation directions allowing pure mode propagation are [100], [111], [110], and all directions which are equivalent to one of these three because of the symmetry of the crystal. Consequently, in the search for useful interactions in cubic crystals, the first interactions considered were interactions for which the two input wave propagation directions were each equivalent to one of the three directions just mentioned. This is not as large a restriction as one might imagine since there are six [100] type directions, eight [111] type directions, and twelve [110] type directions and since there are three possible polarizations for each propagation direction. Some interactions utilizing other propagation directions were investigated and, in fact, some of these others were chosen as "useful" interactions.

The usefulness of an interaction also depends on the linear combination of third order elastic constants appearing in the expression for G, Equation (79). One would like to reduce the amount of calculation necessary for determining a value for a particular elastic constant from measured quantities, thereby reducing the uncertainty in the calculated value. Ideally, each interaction would yield a value for a single third

order elastic constant. In order to apply this criterion for useful interactions a computer program was written to perform the sum,

$$\sum_{rstuvw} C_{rstuvw} \hat{P}^1_r \hat{P}^2_t \hat{P}^3_v \hat{q}^1_s \hat{q}^2_u \hat{q}^3_w \quad ,$$

for each allowed interaction found by the iteration scheme. By means of this program, interactions were chosen which depend on a minimum number of elastic constants.

The chosen useful interactions for copper, gold, silicon, sodium chloride, potassium chloride, and germanium are given in Tables 13 through 18. These tables list the propagation and polarization directions, $\hat{q}$ and $\hat{P}$, for each of the waves involved in the interaction. The quantity μ is defined in Equation (21) and is related to the sound speed, C, by the equation

$$C = \sqrt{\mu/\rho} \quad . \tag{101}$$

The quantities $\frac{\omega_2}{\omega_1}$ and $\frac{\omega_3}{\omega_1}$ are the ratios of the angular frequencies of the waves involved. The final quantity in each tabulation, G, is given by Equation (79) and is expressed as the sum of a linear combination of third order elastic constants and a number, which is calculated from known values of the second order elastic constants. Thus, the tables give enough information about the interaction to allow one who wishes to do the experiment to know in advance what he is measuring and, by means of Equation (95), to evaluate his results.

Since the elastic constant C_{111} is conveniently measured by means of the pulse harmonic distortion experiments, no attempt has been made

to find interactions measuring it. Instead, in choosing useful interactions it is assumed that a value of C_{111} is known and all attention has been concentrated on the remaining five third order elastic constants.

Finally, since one measures the amplitude of the scattered wave, but not its phase relative to the scattering waves, one needs to be able to determine the sign of the quantity G by some other method. This can be done by over-determining the quantities one wishes to calculate. Thus, instead of five useful interactions for the elastic constants to be measured, ten were needed. The purpose of the next section is to show, by means of a sample calculation, how the results of the measurements for the chosen interactions could be used to calculate the values of the elastic constants.

Calculating the Elastic Constants

In order to show how the chosen interactions can be used to measure third order elastic constants, the value of the quantity G for ten of the interactions has been calculated using the elastic constants for copper. These values for G will now be used to recalculate the third order elastic constants along with an estimate of the uncertainty in the calculated value. The values of the elastic constants used in these calculations are those obtained by Granato and Hiki (12) and are given in Table 19. A maximum uncertainty of ± 5 per cent is assigned to the value of G and used to find a maximum uncertainty in the calculated value of the third order elastic constant.

Since the suggested experiment does not measure the sign of G, but only its absolute value, the value of each elastic constant is over-determined, allowing one to choose between the plus or minus signs. The

first two interactions can be used to calculate a value for C_{166}. By using the calculated values for G, one obtains

$$\left| - 0.544\ C_{166} - 0.468 \times 10^{12} \right| = 3.77 \times 10^{12}$$

and

$$\left| 0.978\ C_{166} + 1.772 \times 10^{12} \right| = 5.86 \times 10^{12} \quad .$$

These equations can be rewritten without the absolute value sign by using a ± sign:

$$- 0.544\ C_{166} - 0.468 \times 10^{12} = \pm\ 3.77 \times 10^{12}$$

$$0.978\ C_{166} + 1.772 \times 10^{12} = \pm\ 5.86 \times 10^{12} \quad .$$

Here and in the equations that follow, the ± symbol means that the indicated quantity will later be assigned the + sign or the - sign by requiring that the equations used to determine the elastic constant be consistent. The equations for C_{166} can be solved to yield the equalities

$$C_{166} = (- 0.861 \pm 6.94) \times 10^{12}\ \text{dynes/cm}^2$$

and

$$C_{166} = (- 1.814 \pm 5.99) \times 10^{12}\ \text{dynes/cm}^2 \quad .$$

The only choice of signs which makes these equalities consistent is "-" for each case. The calculated value is, of course, just the value given in the table. The calculated uncertainty is 0.30×10^{12} dynes/cm^2.

The value of C_{144} can be calculated by means of the interactions

labeled 5 and 10. One obtains the equations

$$0.426\ C_{144} - 0.425\ C_{166} - 0.200 \times 10^{12} = \pm 3.112 \times 10^{12}$$

and

$$-0.348\ C_{144} + 0.348\ C_{166} + 0.525 \times 10^{12} = \pm 2.180 \times 10^{12} \quad ,$$

which can be solved to give

$$C_{144} - C_{166} = (0.469 \pm 7.328) \times 10^{12}\ \text{dynes/cm}^2$$

and

$$C_{144} - C_{166} = (1.509 \pm 6.264) \times 10^{12}\ \text{dynes/cm}^2 \quad .$$

These equations are consistent only if one chooses the + sign in each case. The uncertainty in the calculated value of C_{144} is 0.61×10^{12} dynes/cm^2.

The value of C_{456} can be calculated by means of the interactions labeled 3 and 11. One obtains

$$-0.351\ C_{144} + 0.231\ C_{166} + 0.403\ C_{456} + 0.266 \times 10^{12} = \pm 1.903 \times 10^{12}$$

and

$$0.004\ C_{144} - 0.577\ C_{166} + 0.382\ C_{456} - 1.080 \times 10^{12} = \pm 3.057 \times 10^{12} \quad ,$$

which can be solved to give

$$C_{456} = (3.77 \pm 4.73) \times 10^{12}\ \text{dynes/cm}^2$$

and

$$C_{456} = (-\ 8.95 \pm 8.00) \times 10^{12}\ \text{dynes/cm}^2 \quad .$$

In this case one uses the - sign in the first equality and the + sign in the second equality. The uncertainty in the calculated value is 0.84×10^{12} dynes/cm^2.

Next, use the interactions labeled 7 and 8 to obtain a value of C_{112}. The original equations are

$$-\ 0.107\ C_{111} + 0.107\ C_{112} + 0.141\ C_{144} + 0.141\ C_{166} + 0.282\ C_{456}$$

$$-\ 0.140 \times 10^{12} = \pm\ 1.030 \times 10^{12}$$

and

$$-\ 0.263\ C_{111} + 0.135\ C_{112} + 0.383\ C_{166} - 0.855 \times 10^{12} = \pm\ 1.59 \times 10^{12} \quad .$$

These yield the equalities

$$C_{112} = (1.40 \pm 9.62) \times 10^{12}\ \text{dynes/cm}^2$$

and

$$C_{112} = (3.78 \pm 10^{12}\ \text{dynes/cm}^2 \quad .$$

In this case the - sign is used in each equation and the estimated uncertainty is 1.40×10^{12} dynes/cm^2.

Finally, the interactions labeled 6 and 14 are used to obtain a value for C_{123}. One obtains the equations

$$- 0.336\ C_{112} + 0.157\ C_{166} + 0.336\ C_{123} - 0.552 \times 10^{12}$$

$$= \pm 0.841 \times 10^{12}$$

and

$$0.194\ C_{112} - 0.090\ C_{166} - 0.194\ C_{123} + 0.318 \times 10^{12} = \pm 0.463 \times 10^{12}$$

which may be solved to give

$$C_{123} = (- 2.90 \pm 2.50) \times 10^{12}\ \text{dynes/cm}^2$$

and

$$C_{123} = (- 2.89 \pm 2.39) \times 10^{12}\ \text{dynes/cm}^2 \quad .$$

The + sign is chosen in each case and the uncertainty is 1.65×10^{12} dynes/cm^2.

To sum up, the suggested interactions can be used to measure the values of the elastic constants C_{166}, C_{144}, C_{456}, C_{112}, and C_{123} with uncertainties which range from about 4 per cent for C_{166} up to 300 per cent for C_{123} and 2000 per cent for C_{144}, where the large relative uncertainties occur for elastic constants which are small. These uncertainties are based on the assumption that one can measure the quantity G with an uncertainty of 5 per cent. One should be cautioned against comparing these figures with probable errors calculated from the results of experiments since those numbers represent the deviation of measured quantities from the mean, whereas the figures given here represent the maximum uncertainty in calculated quantities due to an experimental uncertainty. Hence, the figures given here have a tendency to look much

worse than a "probable error" for the experiment might turn out to be.

3. Concluding Remarks

The purpose of this chapter was to suggest how one can measure the third order elastic constants of cubic crystals by means of ultrasonic beam scattering experiments. It was suggested that a value for a linear combination of elastic constants could be calculated from the results of an experiment measuring the amplitudes of the two scattering (input) waves and the scattered wave.

In the first section of the chapter an expression was derived to relate the third order elastic constants to quantities which could be measured. This expression, Equation (95), relates the amplitudes and frequencies of the three ultrasonic beams to the geometrical parameters of the experiment and a quantity, G, which is a linear combination of second and third order elastic constants. Unfortunately, G is not a simple function of the scattering propagation directions, but instead it depends on all three propagation directions and their polarization directions. Furthermore, not every combination of scattering propagation-polarization directions yields a resonant scattered wave. Thus, Equation (95) is not useful by itself.

The second section of the chapter is devoted to some calculations which were done in order to make Equation (95) useful for interpreting the results of experiments. First, the problem of finding resonant interactions was discussed and an iteration method for finding resonant interactions was described. The method was used to find a large number of resonant interactions and from these, some potentially useful inter-

actions were chosen and tabulated. Finally, a sample calculation was made in order to show how one could use the results of the experiment to calculate third order elastic constants.

One can conclude that it is possible, in theory, to measure the third order elastic constants of cubic crystals by means of ultrasonic beam scattering experiments.

Table 1. Coefficients for the equations of motion for copper. Values of the second order constants used here are:

$C_{11} = 1.684 \times 10^{12}$ dyn/cm^2 $\quad C_{44} = 0.754 \times 10^{12}$ dyn/cm^2 $\quad C_{12} = 1.214 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	$\mu \times 10^{-12}$ (dyn/cm^2)	$\nu = a + b$	
			a	b $\times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	1.684	1.000C111 + 0.000C112 + 0.000C144 + 0.000C166 + 0.000C123 + 0.000C456	5.052
[0.976, 0.155, 0.155]	[0.921, 0.275, 0.275]	1.817	0.727C111 + 0.216C112 + 0.063C144 + 0.955C166 + 0.010C123 + 0.086C456	5.363
[0.976, 0.155, 0.155]	[-0.389, 0.651, 0.651]	0.646	-0.053C111 + 0.070C112 + 0.154C144 + -0.530C166 -0.023C123 + 0.400C456	-0.346
[0.909, 0.295, 0.295]	[0.814, 0.410, 0.410]	2.054	0.409C111 + 0.474C112 + 0.404C144 + 1.986C166 + 0.065C123 + 0.547C456	6.053
[0.909, 0.295, 0.295]	[-0.580, 0.576, 0.576]	0.474	-0.137C111 + 0.222C112 -0.057C144 + -0.148C166 -0.091C123 + 0.253C456	-0.267
[0.811, 0.413, 0.413]	[0.729, 0.484, 0.484]	2.243	0.223C111 + 0.610C112 + 0.863C144 + 2.480C166 + 0.142C123 + 1.157C456	6.672
[0.811, 0.413, 0.413]	[-0.685, 0.515, 0.515]	0.372	-0.152C111 + 0.301C112 -0.279C144 + 0.195C166 -0.151C123 + 0.047C456	-0.145
[0.697, 0.507, 0.507]	[0.653, 0.535, 0.535]	2.347	0.134C111 + 0.659C112 + 1.210C144 + 2.643C166 + 0.201C123 + 1.616C456	7.027
[0.697, 0.507, 0.507]	[-0.757, 0.462, 0.462]	0.358	-0.122C111 + 0.295C112 -0.342C144 + 0.301C166 -0.174C123 + 0.011C456	-0.064
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	2.376	0.111C111 + 0.667C112 + 1.333C144 + 2.667C166 + 0.222C123 + 1.778C456	7.128
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	0.408	-0.079C111 + 0.236C112 + -0.236C144 + 0.236C166 -0.157C123 + 0.157C456	0.000
[0.988, 0.156, 0.000]	[0.955, 0.297, 0.000]	1.756	0.839C111 + 0.130C112 + 0.000C144 + 0.581C166 + 0.000C123 + 0.000C456	5.212
[0.988, 0.156, 0.000]	[-0.297, 0.955, 0.000]	0.682	-0.022C111 + 0.019C112 + 0.000C144 + -0.346C166 + 0.000C123 + 0.000C456	-0.294

[0,941, 0,306, 0,144]	[0,860, 0,457, 0,229]	1.950	0,532C111 + 0,391C112 + 0,140C144 + 1,666C166 + 0,022C123 + 0,191C456	5,742
[0,941, 0,306, 0,144]	[-0,506, 0,826, 0,250]	0,520	-0,092C111 + 0,111C112 + 0,007C144 + -0,261C166 -0,026C123 + 0,119C456	-0,292
[0,941, 0,306, 0,144]	[-0,074,-0,331, 0,941]	0,722	0,001C111 -0,007C112 -0,199C144 + 0,099C166 + 0,006C123 -0,421C456	-0,077
[0,858, 0,437, 0,268]	[0,770, 0,531, 0,353]	2,156	0,303C111 + 0,575C112 + 0,533C144 + 2,360C166 + 0,087C123 + 0,718C456	6,392
[0,858, 0,437, 0,268]	[-0,626, 0,735, 0,261]	0,384	-0,122C111 + 0,191C112 -0,126C144 + 0,026C166 -0,072C123 + 0,037C456	-0,169
[0,858, 0,437, 0,268]	[-0,120,-0,422, 0,899]	0,652	0,007C111 -0,034C112 -0,203C144 + 0,090C166 + 0,028C123 -0,516C456	-0,092
[0,752, 0,547, 0,367]	[0,693, 0,579, 0,429]	2,293	0,178C111 + 0,654C112 + 0,943C144 + 2,633C166 + 0,156C123 + 1,262C456	6,851
[0,752, 0,547, 0,367]	[-0,696, 0,693, 0,190]	0,327	-0,049C111 + 0,172C112 -0,183C144 + 0,147C166 -0,083C123 -0,034C456	-0,074
[0,752, 0,547, 0,367]	[-0,187,-0,430, 0,883]	0,572	0,018C111 -0,083C112 -0,119C144 + 0,020C166 + 0,064C123 -0,495C456	-0,088
[0,634, 0,634, 0,444]	[0,619, 0,619, 0,485]	2,351	0,130C111 + 0,668C112 + 1,192C144 + 2,677C166 + 0,198C123 + 1,592C456	7,046
[0,634, 0,634, 0,444]	[-0,343,-0,343, 0,875]	0,504	0,038C111 -0,148C112 + 0,009C144 + -0,079C166 + 0,110C123 -0,421C456	-0,069
[0,951, 0,309, 0,000]	[0,879, 0,477, 0,000]	1,909	0,547C111 + 0,363C112 + 0,000C144 + 1,551C166 + 0,000C123 + 0,000C456	5,631
[0,951, 0,309, 0,000]	[-0,477, 0,879, 0,000]	0,529	-0,073C111 + 0,067C112 + 0,000C144 + -0,259C166 + 0,000C123 + 0,000C456	-0,289
[0,884, 0,450, 0,126]	[0,803, 0,568, 0,182]	2,085	0,374C111 + 0,566C112 + 0,154C144 + 2,330C166 + 0,025C123 + 0,209C456	6,181
[0,884, 0,450, 0,126]	[-0,590, 0,801, 0,103]	0,380	-0,095C111 + 0,106C112 -0,026C144 + -0,070C166 -0,015C123 + 0,006C456	-0,169
[0,884, 0,450, 0,126]	[-0,087,-0,190, 0,978]	0,727	0,001C111 + -0,006C112 -0,211C144 + 0,099C166 + 0,005C123 -0,442C456	-0,086

[0,787, 0,572, 0,230]	[0,729, 0,618, 0,294]	2,226	0,233C111 + 0,670C112 + 0,501C144 + 2,701C166 + 0,082C123 + 0,672C456		6,647
[0,787, 0,572, 0,230]	[-0,665, 0,742, 0,088]	0,294	-0,047C111 + 0,094C112 -0,065C144 + 0,042C166 + -0,027C123 -0,022C456		-0,070
[0,787, 0,572, 0,230]	[-0,164,-0,260, 0,952]	0,671	0,005C111 -0,030C112 -0,259C144 + 0,111C166 + 0,025C123 -0,618C456		-0,119
[0,672, 0,672, 0,311]	[0,657, 0,657, 0,371]	2,296	0,173C111 + 0,686C112 + 0,814C144 + 2,749C166 + 0,135C123 + 1,089C456		6,873
[0,672, 0,672, 0,311]	[-0,263,-0,263, 0,928]	0,611	0,013C111 -0,067C112 -0,204C144 + 0,065C166 + 0,054C123 -0,623C456		-0,119
[0,891, 0,454, 0,000]	[0,814, 0,581, 0,000]	2,061	0,400C111 + 0,568C112 + 0,000C144 + 2,335C166 + 0,000C123 + 0,000C456		6,114
[0,891, 0,454, 0,000]	[-0,581, 0,814, 0,000]	0,377	-0,088C111 + 0,085C112 + 0,000C144 + -0,095C166 + 0,000C123 + 0,000C456		-0,168
[0,805, 0,585, 0,105]	[0,752, 0,644, 0,143]	2,180	0,275C111 + 0,693C112 + 0,125C144 + 2,794C166 + 0,021C123 + 0,169C456		6,514
[0,805, 0,585, 0,105]	[-0,654, 0,756, 0,036]	0,277	-0,059C111 + 0,064C112 -0,013C144 + -0,002C166 -0,005C123 -0,005C456		-0,067
[0,805, 0,585, 0,105]	[-0,085,-0,120, 0,989]	0,735	0,000C111 -0,004C112 -0,190C144 + 0,089C166 + 0,003C123 -0,392C456		-0,078
[0,694, 0,694, 0,188]	[0,686, 0,686, 0,242]	2,243	0,216C111 + 0,717C112 + 0,377C144 + 2,872C166 + 0,062C123 + 0,506C456		6,717
[0,694, 0,694, 0,188]	[-0,171,-0,171, 0,970]	0,696	0,003C111 -0,018C112 -0,263C144 + 0,116C166 + 0,016C123 -0,588C456		-0,116
[0,809, 0,588, 0,000]	[0,759, 0,651, 0,000]	2,166	0,287C111 + 0,703C112 + 0,000C144 + 2,830C166 + 0,000C123 + 0,000C456		6,476
[0,809, 0,588, 0,000]	[-0,651, 0,759, 0,000]	0,272	-0,058C111 + 0,057C112 + 0,000C144 + -0,013C166 + 0,000C123 + 0,000C456		-0,066
[0,705, 0,705, 0,084]	[0,703, 0,703, 0,113]	2,211	0,243C111 + 0,742C112 + 0,085C144 + 2,970C166 + 0,014C123 + 0,114C456		6,632
[0,705, 0,705, 0,084]	[-0,080,-0,080, 0,994]	0,742	0,000C111 -0,002C112 -0,159C144 + 0,074C166 + 0,002C123 -0,324C456		-0,064
[0,707, 0,707, 0,000]	[0,707, 0,707, 0,000]	2,203	0,250C111 + 0,750C112 + 0,000C144 + 3,000C166 + 0,000C123 + 0,000C456		6,609

Table 2. Coefficients for the equations of motion for gold. Values of the second order constants used here are:

$C_{11} = 1.86 \times 10^{12}$ dyn/cm^2 $\quad C_{44} = 0.420 \times 10^{12}$ dyn/cm^2 $\quad C_{12} = 1.57 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	$\mu \times 10^{-12}$ (dyn/cm^2)	$\nu = a + b$	
			a	$b \times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	1.860	1.000C111 + 0.000C112 + 0.000C144 + 0.000C166 + 0.000C123 + 0.000C456	5.580
[0.976, 0.155, 0.155]	[0.958, 0.203, 0.203]	1.918	0.817C111 + 0.170C112 + 0.034C144 + 0.695C166 + 0.006C123 + 0.045C456	5.741
[0.976, 0.155, 0.155]	[-0.287, 0.677, 0.677]	0.375	-0.020C111 + 0.038C112 + 0.202C144 + -0.373C166 -0.018C123 + 0.478C456	-0.080
[0.909, 0.295, 0.295]	[0.868, 0.351, 0.351]	2.040	0.493C111 + 0.444C112 + 0.307C144 + 1.798C166 + 0.051C123 + 0.411C456	6.097
[0.909, 0.295, 0.295]	[-0.496, 0.614, 0.614]	0.288	-0.080C111 + 0.168C112 + 0.006C144 + -0.131C166 -0.089C123 + 0.368C456	-0.076
[0.811, 0.413, 0.413]	[0.771, 0.451, 0.451]	2.148	0.257C111 + 0.606C112 + 0.783C144 + 2.434C166 + 0.130C123 + 1.046C456	6.430
[0.811, 0.413, 0.413]	[-0.637, 0.545, 0.545]	0.226	-0.115C111 + 0.272C112 -0.272C144 + 0.219C166 -0.157C123 + 0.086C456	-0.045
[0.697, 0.507, 0.507]	[0.674, 0.522, 0.522]	2.209	0.141C111 + 0.660C112 + 1.186C144 + 2.642C166 + 0.198C123 + 1.582C456	6.625
[0.697, 0.507, 0.507]	[-0.738, 0.477, 0.477]	0.212	-0.108C111 + 0.289C112 -0.358C144 + 0.336C166 -0.180C123 + 0.005C456	-0.020
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	2.227	0.111C111 + 0.667C112 + 1.333C144 + 2.667C166 + 0.222C123 + 1.778C456	6.680
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	0.237	-0.079C111 + 0.236C112 -0.236C144 + 0.236C166 -0.157C123 + 0.157C456	0.000
[0.988, 0.156, 0.000]	[0.978, 0.209, 0.000]	1.891	0.901C111 + 0.095C112 + 0.000C144 + 0.388C166 + 0.000C123 + 0.000C456	5.664
[0.988, 0.156, 0.000]	[-0.209, 0.978, 0.000]	0.389	-0.005C111 + 0.005C112 + 0.000C144 + -0.141C166 + 0.000C123 + 0.000C456	-0.063

[0,941, 0,306, 0,144]	[0,909, 0,375, 0,181]	1,985	0,628C111 + 0,346C112 + 0,093C144 + 1,404C166 + 0,015C123 + 0,125C456	5,935
[0,941, 0,306, 0,144]	[-0,411, 0,878, 0,244]	0,311	-0,038C111 + 0,060C112 + 0,028C144 + -0,168C166 -0,022C123 + 0,144C456	-0,077
[0,941, 0,306, 0,144]	[-0,068,-0,296, 0,953]	0,403	0,002C111 -0,006C112 -0,189C144 + 0,141C166 + 0,005C123 -0,396C456	-0,021
[0,858, 0,437, 0,268]	[0,817, 0,486, 0,309]	2,099	0,356C111 + 0,562C112 + 0,447C144 + 2,262C166 + 0,074C123 + 0,598C456	6,279
[0,858, 0,437, 0,268]	[-0,565, 0,782, 0,264]	0,234	-0,074C111 + 0,144C112 -0,109C144 + 0,046C166 -0,070C123 + 0,062C456	-0,051
[0,858, 0,437, 0,268]	[-0,113,-0,390, 0,914]	0,367	0,009C111 -0,033C112 -0,208C144 + 0,152C166 + 0,024C123 + -0,514C456	-0,026
[0,752, 0,547, 0,367]	[0,722, 0,565, 0,398]	2,179	0,193C111 + 0,656C112 + 0,887C144 + 2,629C166 + 0,147C123 + 1,183C456	6,529
[0,752, 0,547, 0,367]	[-0,668, 0,719, 0,192]	0,196	-0,066C111 + 0,149C112 -0,187C144 + 0,166C166 + -0,083C123 -0,039C456	-0,023
[0,752, 0,547, 0,367]	[-0,178,-0,405, 0,897]	0,325	0,023C111 -0,081C112 -0,134C144 + 0,084C166 + 0,059C123 + -0,502C456	-0,025
[0,634, 0,634, 0,444]	[0,626, 0,626, 0,465]	2,212	0,134C111 + 0,671C112 + 1,170C144 + 2,684C166 + 0,195C123 + 1,561C456	6,636
[0,634, 0,634, 0,444]	[-0,329,-0,329, 0,885]	0,288	0,043C111 -0,145C112 -0,010C144 + -0,026C166 + 0,102C123 -0,430C456	-0,020
[0,951, 0,309, 0,000]	[0,923, 0,384, 0,000]	1,965	0,679C111 + 0,311C112 + 0,000C144 + 1,264C166 + 0,000C123 + 0,000C456	5,878
[0,951, 0,309, 0,000]	[-0,384, 0,923, 0,000]	0,315	-0,025C111 + 0,025C112 + 0,000C144 + -0,138C166 + 0,000C123 + 0,000C456	-0,075
[0,884, 0,450, 0,126]	[0,847, 0,510, 0,152]	2,062	0,431C111 + 0,540C112 + 0,119C144 + 2,178C166 + 0,020C123 + 0,159C456	6,168
[0,884, 0,450, 0,126]	[-0,526, 0,844, 0,101]	0,232	-0,046C111 + 0,059C112 -0,022C144 + -0,040C166 -0,014C123 + 0,011C456	-0,050
[0,884, 0,450, 0,126]	[-0,077,-0,165, 0,983]	0,407	0,001C111 -0,005C112 -0,189C144 + 0,137C166 + 0,004C123 -0,393C456	-0,022

[0.787, 0.572, 0.230]	[0.758, 0.598, 0.261]	2.143	0.253C111 + 0.670C112 + 0.441C144 + 2.686C166 + 0.073C123 + 0.589C456	6.420
[0.787, 0.572, 0.230]	[-0.635, 0.767, 0.088]	0.180	-0.040C111 + 0.067C112 -0.066C144 + 0.052C166 -0.027C123 -0.025C456	-0.022
[0.787, 0.572, 0.230]	[-0.147,-0.232, 0.961]	0.378	0.007C111 -0.027C112 -0.247C144 + 0.176C166 + 0.020C123 -0.576C456	-0.032
[0.672, 0.672, 0.311]	[0.665, 0.665, 0.340]	2.182	0.180C111 + 0.692C112 + 0.761C144 + 2.770C166 + 0.127C123 + 1.016C456	6.543
[0.672, 0.672, 0.311]	[-0.241,-0.241, 0.940]	0.346	0.016C111 -0.062C112 -0.210C144 + 0.141C166 + 0.046C123 -0.603C456	-0.033
[0.891, 0.454, 0.000]	[0.856, 0.517, 0.000]	2.049	0.457C111 + 0.536C112 + 0.000C144 + 2.158C166 + 0.000C123 + 0.000C456	6.132
[0.891, 0.454, 0.000]	[-0.517, 0.856, 0.000]	0.231	-0.039C111 + 0.039C112 + 0.000C144 + -0.060C166 + 0.000C123 + 0.000C456	-0.050
[0.805, 0.585, 0.105]	[0.778, 0.616, 0.122]	2.119	0.292C111 + 0.687C112 + 0.105C144 + 2.755C166 + 0.017C123 + 0.140C456	6.351
[0.805, 0.585, 0.105]	[-0.624, 0.781, 0.036]	0.170	-0.031C111 + 0.036C112 -0.013C144 + 0.003C166 -0.005C123 -0.006C456	-0.021
[0.805, 0.585, 0.105]	[-0.074,-0.104, 0.992]	0.411	0.001C111 -0.003C112 -0.166C144 + 0.120C166 + 0.002C123 -0.342C456	-0.020
[0.694, 0.694, 0.188]	[0.691, 0.691, 0.213]	2.155	0.221C111 + 0.723C112 + 0.334C144 + 2.892C166 + 0.055C123 + 0.446C456	6.462
[0.694, 0.694, 0.188]	[-0.151,-0.151, 0.977]	0.391	0.004C111 -0.016C112 -0.242C144 + 0.173C166 + 0.012C123 -0.531C456	-0.030
[0.809, 0.588, 0.000]	[0.784, 0.621, 0.000]	2.112	0.304C111 + 0.694C112 + 0.000C144 + 2.780C166 + 0.000C123 + 0.000C456	6.331
[0.809, 0.588, 0.000]	[-0.621, 0.784, 0.000]	0.168	-0.029C111 + 0.029C112 + 0.000C144 + -0.009C166 + 0.000C123 + 0.000C456	-0.021
[0.705, 0.705, 0.084]	[0.704, 0.704, 0.097]	2.139	0.244C111 + 0.744C112 + 0.072C144 + 2.976C166 + 0.012C123 + 0.097C456	6.417
[0.705, 0.705, 0.084]	[-0.069,-0.069, 0.995]	0.414	0.000C111 -0.002C112 -0.138C144 + 0.100C166 + 0.001C123 -0.281C456	-0.016
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	2.135	0.250C111 + 0.750C112 + 0.000C144 + 3.000C166 + 0.000C123 + 0.000C456	6.405

Table 3 . Coefficients for the equations of motion for germanium. Values of the second order constants used here are:

$C_{11} = 1.289 \times 10^{12}$ dyn/cm^2 $\quad C_{44} = 0.671 \times 10^{12}$ dyn/cm^2 $\quad C_{12} = 0.483 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	$\mu \times 10^{-12}$ (dyn/cm^2)	$\nu = a + b$	
			a	b $\times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	1.289	1.000C111 + 0.000C112 + 0.000C144 + 0.000C166 + 0.000C123 + 0.000C456	3.867
[0.976, 0.155, 0.155]	[0.933, 0.254, 0.254]	1.354	0.756C111 + 0.204C112 + 0.053C144 + 0.876C166 + 0.008C123 + 0.072C456	4.019
[0.976, 0.155, 0.155]	[-0.359, 0.660, 0.660]	0.619	-0.041C111 + 0.059C112 + 0.168C144 + -0.490C166 -0.022C123 + 0.424C456	-0.271
[0.909, 0.295, 0.295]	[0.839, 0.395, 0.395]	1.476	0.432C111 + 0.468C112 + 0.378C144 + 1.941C166 + 0.061C123 + 0.510C456	4.370
[0.909, 0.295, 0.295]	[-0.558, 0.587, 0.587]	0.531	-0.120C111 + 0.207C112 -0.042C144 + -0.147C166 -0.091C123 + 0.282C456	-0.256
[0.811, 0.413, 0.413]	[0.749, 0.476, 0.476]	1.576	0.231C111 + 0.610C112 + 0.843C144 + 2.471C166 + 0.139C123 + 1.130C456	4.696
[0.811, 0.413, 0.413]	[-0.673, 0.523, 0.523]	0.476	-0.142C111 + 0.294C112 -0.279C144 + 0.200C166 -0.153C123 + 0.056C456	-0.162
[0.697, 0.507, 0.507]	[0.659, 0.532, 0.532]	1.631	0.146C111 + 0.659C112 + 1.205C144 + 2.643C166 + 0.200C123 + 1.608C456	4.885
[0.697, 0.507, 0.507]	[-0.753, 0.466, 0.466]	0.467	-0.118C111 + 0.294C112 -0.346C144 + 0.310C166 -0.175C123 + 0.009C456	-0.074
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	1.646	0.111C111 + 0.667C112 + 1.333C144 + 2.667C166 + 0.222C123 + 1.778C456	4.939
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	0.492	-0.079C111 + 0.236C112 -0.236C144 + 0.236C166 -0.157C123 + 0.157C456	0.000
[0.988, 0.156, 0.000]	[0.963, 0.269, 0.000]	1.324	0.861C111 + 0.119C112 + 0.000C144 + 0.517C166 + 0.000C123 + 0.000C456	3.945
[0.988, 0.156, 0.000]	[-0.269, 0.963, 0.000]	0.636	-0.015C111 + 0.014C112 + 0.000C144 + -0.286C166 + 0.000C123 + 0.000C456	-0.220

[0.941, 0.306, 0.144]	[0.874, 0.435, 0.215]	1.422	0.560C111 + 0.381C112 + 0.126C144 + 1.597C166 + 0.020C123 + 0.171C456		4.210
[0.941, 0.306, 0.144]	[-0.480, 0.841, 0.250]	0.555	-0.075C111 + 0.096C112 + 0.013C144 + -0.242C166 -0.025C123 + 0.127C456		-0.263
[0.941, 0.306, 0.144]	[-0.073,-0.321, 0.944]	0.654	0.001C111 -0.007C112 -0.196C144 + 0.111C166 + 0.005C123 -0.415C456		-0.060
[0.858, 0.437, 0.268]	[0.783, 0.520, 0.341]	1.530	0.316C111 + 0.573C112 + 0.511C144 + 2.338C166 + 0.084C123 + 0.686C456		4.549
[0.858, 0.437, 0.268]	[-0.611, 0.747, 0.262]	0.482	-0.109C111 + 0.179C112 -0.122C144 + 0.030C166 -0.072C123 + 0.043C456		-0.184
[0.858, 0.437, 0.268]	[-0.119,-0.413, 0.903]	0.619	0.007C111 -0.034C112 -0.204C144 + 0.106C166 + 0.027C123 -0.516C456		-0.076
[0.752, 0.547, 0.367]	[0.701, 0.576, 0.421]	1.603	0.182C111 + 0.655C112 + 0.929C144 + 2.634C166 + 0.154C123 + 1.243C456		4.793
[0.752, 0.547, 0.367]	[-0.689, 0.699, 0.190]	0.451	-0.083C111 + 0.166C112 -0.184C144 + 0.151C166 -0.083C123 -0.036C456		-0.090
[0.752, 0.547, 0.367]	[-0.185,-0.423, 0.887]	0.577	0.020C111 -0.083C112 -0.123C144 + 0.036C166 + 0.063C123 -0.497C456		-0.077
[0.634, 0.634, 0.444]	[0.620, 0.620, 0.480]	1.633	0.131C111 + 0.669C112 + 1.187C144 + 2.679C166 + 0.198C123 + 1.584C456		4.896
[0.634, 0.634, 0.444]	[-0.339,-0.339, 0.877]	0.542	0.039C111 -0.147C112 + 0.004C144 + -0.066C166 + 0.108C123 -0.423C456		-0.065
[0.951, 0.309, 0.000]	[0.893, 0.451, 0.000]	1.401	0.614C111 + 0.351C112 + 0.000C144 + 1.472C166 + 0.000C123 + 0.000C456		4.154
[0.951, 0.309, 0.000]	[-0.451, 0.893, 0.000]	0.559	-0.058C111 + 0.054C112 + 0.000C144 + -0.231C166 + 0.000C123 + 0.000C456		-0.256
[0.884, 0.450, 0.126]	[0.815, 0.553, 0.174]	1.493	0.389C111 + 0.561C112 + 0.145C144 + 2.295C166 + 0.024C123 + 0.195C456		4.440
[0.884, 0.450, 0.126]	[-0.574, 0.813, 0.102]	0.480	-0.081C111 + 0.094C112 -0.025C144 + -0.065C166 -0.014C123 + 0.007C456		-0.185
[0.884, 0.450, 0.126]	[-0.084,-0.183, 0.979]	0.657	0.001C111 -0.006C112 -0.205C144 + 0.110C166 + 0.005C123 -0.429C456		-0.066

[0.787, 0.572, 0.230]	[0.736, 0.613, 0.285]	1.568	0.238C111 + 0.670C112 + 0.485C144 + 2.699C166 + 0.080C123 + 0.650C456		4.686
[0.787, 0.572, 0.230]	[-0.657, 0.748, 0.088]	0.434	-0.060C111 + 0.087C112 -0.065C144 + 0.044C166 -0.027C123 -0.023C456		-0.090
[0.787, 0.572, 0.230]	[-0.159,-0.253, 0.954]	0.629	0.006C111 -0.030C112 -0.256C144 + 0.129C166 + 0.024C123 -0.607C456		-0.096
[0.672, 0.672, 0.311]	[0.659, 0.659, 0.363]	1.604	0.175C111 + 0.687C112 + 0.800C144 + 2.755C166 + 0.133C123 + 1.070C456		4.806
[0.672, 0.672, 0.311]	[-0.257,-0.257, 0.932]	0.598	0.014C111 -0.066C112 -0.206C144 + 0.046C166 + 0.052C123 -0.619C456		-0.100
[0.891, 0.454, 0.000]	[0.825, 0.565, 0.000]	1.481	0.415C111 + 0.561C112 + 0.000C144 + 2.299C166 + 0.000C123 + 0.000C456		4.406
[0.891, 0.454, 0.000]	[-0.565, 0.825, 0.000]	0.479	-0.075C111 + 0.073C112 + 0.000C144 + -0.088C166 + 0.000C123 + 0.000C456		-0.184
[0.805, 0.585, 0.105]	[0.759, 0.637, 0.137]	1.544	0.279C111 + 0.693C112 + 0.120C144 + 2.786C166 + 0.020C123 + 0.161C456		4.619
[0.805, 0.585, 0.105]	[-0.646, 0.762, 0.036]	0.425	-0.052C111 + 0.057C112 -0.013C144 + -0.001C166 -0.005C123 -0.006C456		-0.090
[0.805, 0.585, 0.105]	[-0.082,-0.116, 0.990]	0.661	0.001C111 -0.003C112 -0.183C144 + 0.097C166 + 0.003C123 -0.378C456		-0.059
[0.694, 0.694, 0.188]	[0.687, 0.687, 0.234]	1.577	0.218C111 + 0.719C112 + 0.365C144 + 2.878C166 + 0.060C123 + 0.489C456		4.726
[0.694, 0.694, 0.188]	[-0.166,-0.166, 0.972]	0.641	0.003C111 -0.018C112 -0.257C144 + 0.132C166 + 0.015C123 -0.573C456		-0.091
[0.809, 0.588, 0.000]	[0.765, 0.644, 0.000]	1.537	0.292C111 + 0.701C112 + 0.000C144 + 2.819C166 + 0.000C123 + 0.000C456		4.599
[0.809, 0.588, 0.000]	[-0.644, 0.765, 0.000]	0.423	-0.050C111 + 0.050C112 + 0.000C144 + -0.012C166 + 0.000C123 + 0.000C456		-0.090
[0.705, 0.705, 0.084]	[0.703, 0.703, 0.108]	1.561	0.243C111 + 0.743C112 + 0.081C144 + 2.972C166 + 0.013C123 + 0.109C456		4.682
[0.705, 0.705, 0.084]	[-0.077,-0.077, 0.994]	0.665	0.000C111 -0.002C112 -0.153C144 + 0.041C166 + 0.001C123 -0.312C456		-0.049
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	1.557	0.250C111 + 0.750C112 + 0.000C144 + 3.000C166 + 0.000C123 + 0.000C456		4.671

Table 4. Coefficients for the equations of motion for silicon. Values of the second order constants used here are:

$C_{11} = 1.657 \times 10^{12}$ dyn/cm^2 $\quad C_{44} = 0.796 \times 10^{12}$ dyn/cm^2 $\quad C_{12} = 0.639 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	$\mu \times 10^{-12}$ (dyn/cm^2)	$\nu = a + b$	
			a	$b \times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	1.657	1.000C111 + 0.000C112 + 0.000C144 + 0.000C166 + 0.000C123 + 0.000C456	4.971
[0.976, 0.155, 0.155]	[0.944, 0.234, 0.234]	1.723	0.781C111 + 0.192C112 + 0.045C144 + 0.805C166 + 0.007C123 + 0.061C456	5.134
[0.976, 0.155, 0.155]	[-0.331, 0.667, 0.667]	0.743	-0.032C111 + 0.051C112 + 0.181C144 + -0.449C166 -0.021C123 + 0.445C456	-0.261
[0.909, 0.295, 0.295]	[0.844, 0.379, 0.379]	1.853	0.454C111 + 0.461C112 + 0.352C144 + 1.893C166 + 0.058C123 + 0.474C456	5.508
[0.909, 0.295, 0.295]	[-0.536, 0.597, 0.597]	0.650	-0.105C111 + 0.193C112 -0.026C144 + -0.144C166 -0.091C123 + 0.312C456	-0.263
[0.811, 0.413, 0.413]	[0.751, 0.467, 0.467]	1.962	0.240C111 + 0.609C112 + 0.823C144 + 2.460C166 + 0.136C123 + 1.101C456	5.857
[0.811, 0.413, 0.413]	[-0.661, 0.531, 0.531]	0.589	-0.133C111 + 0.287C112 -0.277C144 + 0.206C166 -0.155C123 + 0.065C456	-0.172
[0.697, 0.507, 0.507]	[0.664, 0.529, 0.529]	2.022	0.138C111 + 0.660C112 + 1.198C144 + 2.643C166 + 0.199C123 + 1.599C456	6.061
[0.697, 0.507, 0.507]	[-0.743, 0.470, 0.470]	0.578	-0.115C111 + 0.292C112 -0.350C144 + 0.319C166 -0.177C123 + 0.008C456	-0.079
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	2.040	0.111C111 + 0.667C112 + 1.333C144 + 2.667C166 + 0.222C123 + 1.778C456	6.119
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	0.605	-0.079C111 + 0.236C112 -0.236C144 + 0.236C166 -0.157C123 + 0.157C456	0.000
[0.988, 0.156, 0.000]	[0.969, 0.246, 0.000]	1.692	0.878C111 + 0.110C112 + 0.000C144 + 0.464C166 + 0.000C123 + 0.000C456	5.055
[0.988, 0.156, 0.000]	[-0.246, 0.969, 0.000]	0.761	-0.011C111 + 0.010C112 + 0.000C144 + -0.230C166 + 0.000C123 + 0.000C456	-0.208

[0,941, 0,306, 0,144]	[0,884, 0,413, 0,203]	1,795	0,585C111 + 0,370C112 + 0,114C144 + 1,528C166 + 0,018C123 + 0,153C456	5,338
[0,941, 0,306, 0,144]	[-0,455, 0,855, 0,248]	0,675	-0,060C111 + 0,082C112 + 0,019C144 + -0,219C166 -0,024C123 + 0,134C456	-0,264
[0,941, 0,306, 0,144]	[-0,071,-0,312, 0,947]	0,778	0,001C111 -0,007C112 -0,194C144 + 0,122C166 + 0,005C123 -0,408C456	-0,060
[0,858, 0,437, 0,268]	[0,795, 0,509, 0,330]	1,912	0,330C111 + 0,570C112 + 0,488C144 + 2,314C166 + 0,080C123 + 0,655C456	5,699
[0,858, 0,437, 0,268]	[-0,595, 0,760, 0,263]	0,597	-0,096C111 + 0,167C112 -0,118C144 + 0,034C166 -0,072C123 + 0,050C456	-0,194
[0,858, 0,437, 0,268]	[-0,117,-0,405, 0,907]	0,740	0,008C111 -0,034C112 -0,206C144 + 0,122C166 + 0,026C123 -0,515C456	-0,077
[0,752, 0,547, 0,367]	[0,708, 0,572, 0,413]	1,992	0,186C111 + 0,656C112 + 0,915C144 + 2,633C166 + 0,152C123 + 1,222C456	5,961
[0,752, 0,547, 0,367]	[-0,682, 0,706, 0,191]	0,561	-0,077C111 + 0,160C112 -0,185C144 + 0,156C166 -0,083C123 -0,037C456	-0,096
[0,752, 0,547, 0,367]	[-0,182,-0,417, 0,890]	0,696	0,021C111 -0,082C112 -0,127C144 + 0,053C166 + 0,061C123 -0,499C456	-0,079
[0,634, 0,634, 0,444]	[0,622, 0,622, 0,475]	2,025	0,132C111 + 0,670C112 + 1,181C144 + 2,681C166 + 0,197C123 + 1,576C456	6,072
[0,634, 0,634, 0,444]	[-0,336,-0,336, 0,880]	0,658	0,041C111 -0,147C112 -0,001C144 + -0,052C166 + 0,106C123 -0,426C456	-0,067
[0,951, 0,309, 0,000]	[0,905, 0,426, 0,000]	1,773	0,639C111 + 0,337C112 + 0,000C144 + 1,396C166 + 0,000C123 + 0,000C456	5,278
[0,951, 0,309, 0,000]	[-0,426, 0,905, 0,000]	0,680	-0,045C111 + 0,043C112 + 0,000C144 + -0,200C166 + 0,000C123 + 0,000C456	-0,256
[0,884, 0,450, 0,126]	[0,826, 0,538, 0,166]	1,873	0,404C111 + 0,555C112 + 0,135C144 + 2,256C166 + 0,022C123 + 0,182C456	5,583
[0,884, 0,450, 0,126]	[-0,557, 0,824, 0,102]	0,595	-0,068C111 + 0,081C112 -0,024C144 + -0,058C166 -0,014C123 + 0,009C456	-0,193
[0,884, 0,450, 0,126]	[-0,082,-0,177, 0,981]	0,782	0,001C111 -0,005C112 -0,199C144 + 0,120C166 + 0,004C123 -0,416C456	-0,065

[0.787, 0.572, 0.230]	[0.744, 0.608, 0.276]	1.954	0.244C111 + 0.671C112 + 0.469C144 + 2.696C166 + 0.078C123 + 0.628C456		5.848
[0.787, 0.572, 0.230]	[-0.650, 0.755, 0.088]	0.544	-0.053C111 + 0.080C112 -0.066C144 + 0.047C166 -0.027C123 -0.024C456		-0.097
[0.787, 0.572, 0.230]	[-0.155,-0.245, 0.957]	0.751	0.006C111 -0.029C112 -0.253C144 + 0.146C166 + 0.023C123 -0.596C456		-0.096
[0.672, 0.672, 0.311]	[0.661, 0.661, 0.355]	1.994	0.177C111 + 0.689C112 + 0.787C144 + 2.761C166 + 0.131C123 + 1.051C456		5.976
[0.672, 0.672, 0.311]	[-0.251,-0.251, 0.935]	0.718	0.015C111 -0.065C112 -0.207C144 + 0.106C166 + 0.050C123 -0.613C456		-0.102
[0.891, 0.454, 0.000]	[0.837, 0.548, 0.000]	1.860	0.429C111 + 0.553C112 + 0.000C144 + 2.247C166 + 0.000C123 + 0.000C456		5.546
[0.891, 0.454, 0.000]	[-0.548, 0.837, 0.000]	0.593	-0.062C111 + 0.060C112 + 0.000C144 + -0.080C166 + 0.000C123 + 0.000C456		-0.193
[0.805, 0.585, 0.105]	[0.766, 0.630, 0.132]	1.929	0.284C111 + 0.691C112 + 0.114C144 + 2.776C166 + 0.019C123 + 0.153C456		5.775
[0.805, 0.585, 0.105]	[-0.638, 0.769, 0.036]	0.534	-0.045C111 + 0.050C112 -0.013C144 + 0.000C166 -0.005C123 -0.006C456		-0.097
[0.805, 0.585, 0.105]	[-0.079,-0.112, 0.991]	0.786	0.001C111 -0.003C112 -0.177C144 + 0.106C166 + 0.003C123 -0.365C456		-0.058
[0.694, 0.694, 0.188]	[0.689, 0.689, 0.227]	1.965	0.219C111 + 0.720C112 + 0.354C144 + 2.883C166 + 0.059C123 + 0.473C456		5.891
[0.694, 0.694, 0.188]	[-0.160,-0.160, 0.974]	0.765	0.003C111 -0.017C112 -0.252C144 + 0.147C166 + 0.014C123 -0.558C456		-0.091
[0.809, 0.588, 0.000]	[0.772, 0.636, 0.000]	1.922	0.296C111 + 0.699C112 + 0.000C144 + 2.806C166 + 0.000C123 + 0.000C456		5.755
[0.809, 0.588, 0.000]	[-0.636, 0.772, 0.000]	0.531	-0.043C111 + 0.043C112 + 0.000C144 + -0.011C166 + 0.000C123 + 0.000C456		-0.097
[0.705, 0.705, 0.084]	[0.703, 0.703, 0.104]	1.948	0.243C111 + 0.743C112 + 0.078C144 + 2.973C166 + 0.013C123 + 0.104C456		5.844
[0.705, 0.705, 0.084]	[-0.074,-0.074, 0.995]	0.789	0.000C111 -0.002C112 -0.148C144 + 0.098C166 + 0.001C123 -0.301C456		-0.048
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	1.944	0.250C111 + 0.750C112 + 0.000C144 + 3.000C166 + 0.000C123 + 0.000C456		5.832

Table 5. Coefficients for the equations of motion for potassium chloride. Values of the second order constants used here are:

$C_{11} = 0.398 \times 10^{12}$ dyn/cm^2 $\quad C_{44} = 0.00625 \times 10^{12}$ dyn/cm^2 $\quad C_{12} = 0.062 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	$\mu \times 10^{-12}$ (dyn/cm^2)	$\nu = a + b$	
			a	b $\times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	0.398	1.000C111 + 0.000C112 + 0.000C144 + 0.000C166 + 0.000C123 + 0.000C456	1.194
[0.976, 0.155, 0.155]	[0.999, 0.028, 0.028]	0.380	0.927C111 + 0.025C112 + 0.001C144 + 0.195C166 + 0.000C123 + 0.002C456	1.121
[0.976, 0.155, 0.155]	[-0.040, 0.707, 0.707]	0.017	0.003C111 + 0.006C112 + 0.300C144 + 0.227C166 -0.003C123 + 0.612C456	0.009
[0.909, 0.295, 0.295]	[0.996, 0.064, 0.064]	0.332	0.741C111 + 0.095C112 + 0.018C144 + 0.687C166 + 0.002C123 + 0.028C456	0.939
[0.909, 0.295, 0.295]	[-0.090, 0.704, 0.704]	0.044	0.017C111 + 0.041C112 + 0.427C144 + 0.500C166 -0.021C123 + 0.938C456	0.044
[0.811, 0.413, 0.413]	[0.985, 0.122, 0.122]	0.270	0.511C111 + 0.206C112 + 0.102C144 + 1.309C166 + 0.012C123 + 0.155C456	0.728
[0.811, 0.413, 0.413]	[-0.172, 0.697, 0.697]	0.079	0.045C111 + 0.107C112 + 0.282C144 + 0.789C166 -0.070C123 + 0.843C456	0.104
[0.697, 0.507, 0.507]	[0.930, 0.261, 0.261]	0.210	0.277C111 + 0.415C112 + 0.474C144 + 2.051C166 + 0.068C123 + 0.676C456	0.576
[0.697, 0.507, 0.507]	[-0.369, 0.657, 0.657]	0.111	0.057C111 + 0.183C112 -0.195C144 + 0.990C166 -0.171C123 + 0.295C456	0.136
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	0.182	0.111C111 + 0.667C112 + 1.333C144 + 2.667C166 + 0.222C123 + 1.778C456	0.547
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	0.114	-0.079C111 + 0.236C112 -0.236C144 + 0.236C166 -0.157C123 + 0.157C456	0.000
[0.988, 0.156, 0.000]	[1.000, 0.028, 0.000]	0.389	0.962C111 + 0.013C112 + 0.000C144 + 0.101C166 + 0.000C123 + 0.000C456	1.156
[0.988, 0.156, 0.000]	[-0.028, 1.000, 0.000]	0.016	0.004C111 -0.002C112 + 0.000C144 + 0.372C166 + 0.000C123 + 0.000C456	0.006

[0,941, 0,306, 0,144]	[0,995, 0,063, 0,028]	0,355	0,828C111 + 0,063C112 + 0,004C144 + 0,463C166 + 0,000C123 + 0,007C456	1,024
[0,941, 0,306, 0,144]	[-0,065, 0,994, 0,087]	0,042	0,028C111 -0,010C112 + 0,031C144 + 0,637C166 -0,001C123 + 0,067C456	0,032
[0,941, 0,306, 0,144]	[-0,022,-0,088, 0,996]	0,014	0,003C111 -0,003C112 -0,073C144 + 0,350C166 + 0,000C123 -0,147C456	0,004
[0,858, 0,437, 0,268]	[0,991, 0,119, 0,062]	0,299	0,616C111 + 0,157C112 + 0,039C144 + 1,042C166 + 0,004C123 + 0,061C456	0,825
[0,858, 0,437, 0,268]	[-0,126, 0,983, 0,132]	0,079	0,078C111 -0,023C112 + 0,040C144 + 0,743C166 -0,010C123 + 0,120C456	0,085
[0,858, 0,437, 0,268]	[-0,046,-0,138, 0,989]	0,032	0,018C111 -0,018C112 -0,130C144 + 0,565C166 + 0,004C123 -0,276C456	0,016
[0,752, 0,547, 0,367]	[0,961, 0,250, 0,121]	0,238	0,380C111 + 0,332C112 + 0,203C144 + 1,779C166 + 0,026C123 + 0,300C456	0,645
[0,752, 0,547, 0,367]	[-0,266, 0,954, 0,138]	0,117	0,134C111 -0,051C112 -0,059C144 + 0,628C166 -0,032C123 + 0,009C456	0,131
[0,752, 0,547, 0,367]	[-0,081,-0,165, 0,983]	0,055	0,044C111 -0,049C112 -0,147C144 + 0,627C166 + 0,012C123 -0,341C456	0,035
[0,634, 0,634, 0,444]	[0,688, 0,688, 0,232]	0,197	0,167C111 + 0,642C112 + 0,771C144 + 2,648C166 + 0,117C123 + 1,071C456	0,577
[0,634, 0,634, 0,444]	[-0,164,-0,164, 0,973]	0,077	0,078C111 -0,095C112 -0,128C144 + 0,554C166 + 0,028C123 -0,368C456	0,052
[0,951, 0,309, 0,000]	[0,998, 0,063, 0,000]	0,362	0,855C111 + 0,054C112 + 0,000C144 + 0,394C166 + 0,000C123 + 0,000C456	1,051
[0,951, 0,309, 0,000]	[-0,063, 0,998, 0,000]	0,042	0,029C111 -0,014C112 + 0,000C144 + 0,645C166 + 0,000C123 + 0,000C456	0,032
[0,884, 0,450, 0,126]	[0,993, 0,118, 0,026]	0,316	0,676C111 + 0,138C112 + 0,008C144 + 0,906C166 + 0,001C123 + 0,013C456	0,884
[0,884, 0,450, 0,126]	[-0,119, 0,992, 0,042]	0,083	0,088C111 -0,045C112 + 0,005C144 + 0,723C166 -0,001C123 + 0,016C456	0,086
[0,884, 0,450, 0,126]	[-0,021,-0,045, 0,999]	0,012	0,002C111 -0,002C112 -0,057C144 + 0,311C166 + 0,000C123 -0,115C456	0,003

[0.787, 0.572, 0.230]	[0.967, 0.246, 0.061]	0.258	0.445C111 + 0.316C112 + 0.073C144 + 1.684C166 + 0.009C123 + 0.111C456		0.709
[0.787, 0.572, 0.230]	[-0.249, 0.967, 0.056]	0.127	0.162C111 -0.103C112 -0.023C144 + 0.519C166 -0.008C123 -0.012C456		0.141
[0.787, 0.572, 0.230]	[-0.046,-0.069, 0.997]	0.026	0.012C111 -0.010C112 -0.100C144 + 0.520C166 + 0.002C123 -0.207C456		0.012
[0.672, 0.672, 0.311]	[0.702, 0.702, 0.116]	0.216	0.210C111 + 0.683C112 + 0.345C144 + 2.792C166 + 0.048C123 + 0.497C456		0.636
[0.672, 0.672, 0.311]	[-0.082,-0.082, 0.993]	0.042	0.029C111 -0.027C112 -0.125C144 + 0.623C166 + 0.006C123 -0.273C456		0.025
[0.891, 0.454, 0.000]	[0.993, 0.117, 0.000]	0.321	0.693C111 + 0.133C112 + 0.000C144 + 0.868C166 + 0.000C123 + 0.000C456		0.902
[0.891, 0.454, 0.000]	[-0.117, 0.993, 0.000]	0.084	0.090C111 -0.049C112 + 0.000C144 + 0.718C166 + 0.000C123 + 0.000C456		0.087
[0.805, 0.585, 0.105]	[0.969, 0.244, 0.026]	0.268	0.477C111 + 0.313C112 + 0.015C144 + 1.647C166 + 0.002C123 + 0.023C456		0.744
[0.805, 0.585, 0.105]	[-0.245, 0.969, 0.022]	0.132	0.174C111 -0.121C112 -0.005C144 + 0.473C166 -0.002C123 -0.004C456		0.147
[0.805, 0.585, 0.105]	[-0.020,-0.027, 0.999]	0.010	0.001C111 -0.001C112 -0.047C144 + 0.262C166 + 0.000C123 -0.094C456		0.002
[0.694, 0.694, 0.188]	[0.706, 0.706, 0.060]	0.229	0.236C111 + 0.723C112 + 0.123C144 + 2.918C166 + 0.016C123 + 0.180C456		0.681
[0.694, 0.694, 0.188]	[-0.043,-0.043, 0.998]	0.019	0.007C111 -0.005C112 -0.081C144 + 0.445C166 + 0.001C123 -0.167C456		0.007
[0.809, 0.588, 0.000]	[0.970, 0.244, 0.000]	0.271	0.486C111 + 0.313C112 + 0.000C144 + 1.638C166 + 0.000C123 + 0.000C456		0.754
[0.809, 0.588, 0.000]	[-0.244, 0.970, 0.000]	0.133	0.178C111 -0.126C112 + 0.000C144 + 0.460C166 + 0.000C123 + 0.000C456		0.149
[0.705, 0.705, 0.084]	[0.707, 0.707, 0.025]	0.235	0.247C111 + 0.745C112 + 0.024C144 + 2.983C166 + 0.003C123 + 0.036C456		0.703
[0.705, 0.705, 0.084]	[-0.018,-0.018, 1.000]	0.009	0.001C111 + 0.000C112 -0.037C144 + 0.211C166 + 0.000C123 -0.075C456		0.002
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	0.236	0.250C111 + 0.750C112 + 0.000C144 + 3.000C166 + 0.000C123 + 0.000C456		0.709

Table 6. Coefficients for the equations of motion for sodium chloride. Values of the second order constants used here are:

$C_{11} = 0.487 \times 10^{12}$ dyn/cm^2 $\quad C_{44} = 0.126 \times 10^{12}$ dyn/cm^2 $\quad C_{12} = 0.124 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	$\mu \times 10^{-12}$ (dyn/cm^2)	$\nu = a + b$	
			a	b $\times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	0.487	1.000C111 + 0.000C112 + 0.000C144 + 0.000C166 + 0.000C123 + 0.000C456	1.461
[0.976, 0.155, 0.155]	[0.988, 0.110, 0.110]	0.478	0.895C111 + 0.097C112 + 0.010C144 + 0.399C166 + 0.002C123 + 0.014C456	1.432
[0.976, 0.155, 0.155]	[-0.156, 0.698, 0.698]	0.132	-0.001C111 + 0.012C112 + 0.259C144 + -0.085C166 -0.011C123 + 0.560C456	0.025
[0.909, 0.295, 0.295]	[0.946, 0.229, 0.229]	0.457	0.636C111 + 0.325C112 + 0.143C144 + 1.329C166 + 0.024C123 + 0.193C456	1.363
[0.909, 0.295, 0.295]	[-0.324, 0.669, 0.669]	0.147	-0.010C111 + 0.080C112 + 0.173C144 + 0.033C166 -0.069C123 + 0.622C456	0.044
[0.811, 0.413, 0.413]	[0.863, 0.357, 0.357]	0.433	0.350C111 + 0.545C112 + 0.553C144 + 2.204C166 + 0.092C123 + 0.741C456	1.293
[0.811, 0.413, 0.413]	[-0.505, 0.610, 0.610]	0.161	-0.037C111 + 0.194C112 -0.189C144 + 0.308C166 -0.156C123 + 0.248C456	0.046
[0.697, 0.507, 0.507]	[0.733, 0.481, 0.481]	0.418	0.163C111 + 0.651C112 + 1.095C144 + 2.611C166 + 0.182C123 + 1.461C456	1.251
[0.697, 0.507, 0.507]	[-0.680, 0.518, 0.518]	0.167	-0.071C111 + 0.267C112 -0.392C144 + 0.435C166 -0.196C123 + 0.001C456	0.025
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	0.413	0.111C111 + 0.667C112 + 1.333C144 + 2.667C166 + 0.222C123 + 1.778C456	1.239
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	0.163	-0.079C111 + 0.236C112 -0.236C144 + 0.236C166 -0.157C123 + 0.157C456	0.000
[0.988, 0.156, 0.000]	[0.994, 0.110, 0.000]	0.482	0.946C111 + 0.051C112 + 0.000C144 + 0.210C166 + 0.000C123 + 0.000C456	1.446
[0.988, 0.156, 0.000]	[-0.110, 0.994, 0.000]	0.131	0.002C111 -0.002C112 + 0.000C144 + 0.129C166 + 0.000C123 + 0.000C456	0.018

[0.941, 0.306, 0.144]	[0.967, 0.231, 0.106]	0.467	0.755C111 + 0.228C112 + 0.036C144 + 0.934C166 + 0.006C123 + 0.048C456	1.394
[0.941, 0.306, 0.144]	[-0.248, 0.947, 0.205]	0.143	0.012C111 + 0.001C112 + 0.053C144 + 0.134C166 -0.012C123 + 0.154C456	0.037
[0.941, 0.306, 0.144]	[-0.053,-0.225, 0.973]	0.129	0.002C111 -0.005C112 -0.159C144 + 0.220C166 + 0.003C123 -0.329C456	0.008
[0.858, 0.437, 0.268]	[0.905, 0.367, 0.215]	0.444	0.473C111 + 0.469C112 + 0.261C144 + 1.902C166 + 0.043C123 + 0.350C456	1.325
[0.858, 0.437, 0.268]	[-0.414, 0.875, 0.252]	0.159	0.011C111 + 0.045C112 -0.048C144 + 0.176C166 -0.055C123 + 0.124C456	0.045
[0.858, 0.437, 0.268]	[-0.096,-0.317, 0.944]	0.136	0.013C111 -0.030C112 -0.208C144 + 0.286C166 + 0.017C123 + -0.484C456	0.013
[0.752, 0.547, 0.367]	[0.795, 0.513, 0.323]	0.425	0.238C111 + 0.635C112 + 0.720C144 + 2.552C166 + 0.119C123 + 0.962C456	1.271
[0.752, 0.547, 0.367]	[-0.586, 0.787, 0.193]	0.170	-0.006C111 + 0.087C112 -0.184C144 + 0.226C166 -0.081C123 + -0.045C456	0.031
[0.752, 0.547, 0.367]	[-0.155,-0.342, 0.927]	0.145	0.031C111 -0.076C112 -0.161C144 + 0.235C166 + 0.045C123 -0.501C456	0.016
[0.634, 0.634, 0.444]	[0.644, 0.644, 0.413]	0.416	0.142C111 + 0.473C112 + 1.101C144 + 2.694C166 + 0.183C123 + 1.469C456	1.248
[0.634, 0.634, 0.444]	[-0.292,-0.292, 0.911]	0.152	0.053C111 -0.137C112 -0.056C144 + 0.110C166 + 0.083C123 -0.444C456	0.016
[0.951, 0.309, 0.000]	[0.973, 0.231, 0.000]	0.470	0.793C111 + 0.197C112 + 0.000C144 + 0.810C166 + 0.000C123 + 0.000C456	1.405
[0.951, 0.309, 0.000]	[-0.231, 0.973, 0.000]	0.143	0.017C111 -0.016C112 + 0.000C144 + 0.177C166 + 0.000C123 + 0.000C456	0.035
[0.884, 0.450, 0.126]	[0.924, 0.371, 0.097]	0.451	0.549C111 + 0.428C112 + 0.061C144 + 1.738C166 + 0.010C123 + 0.082C456	1.347
[0.884, 0.450, 0.126]	[-0.379, 0.921, 0.090]	0.160	0.034C111 -0.024C112 -0.009C144 + 0.129C166 -0.009C123 + 0.019C456	0.044
[0.884, 0.450, 0.126]	[-0.056,-0.120, 0.991]	0.128	0.002C111 -0.004C112 -0.144C144 + 0.205C166 + 0.002C123 -0.295C456	0.008
[0.787, 0.572, 0.230]	[0.827, 0.529, 0.191]	0.432	0.304C111 + 0.637C112 + 0.313C144 + 2.560C166 + 0.052C123 + 0.418C456	1.293

[0,787, 0,572, 0,230]	[-0,550, 0,830, 0,086]	0,173	0,026C111 -0,001C112 -0,063C144 + 0,095C166 -0,024C123 -0,029C456	0,032
[0,787, 0,572, 0,230]	[-0,113,-0,176, 0,978]	0,134	0,010C111 -0,022C112 -0,211C144 + 0,302C166 + 0,012C123 -0,471C456	0,014
[0,672, 0,672, 0,311]	[0,681, 0,681, 0,271]	0,423	0,192C111 + 0,700C112 + 0,637C144 + 2,891C166 + 0,106C123 + 0,850C456	1,267
[0,672, 0,672, 0,311]	[-0,192,-0,192, 0,963]	0,140	0,022C111 -0,052C112 -0,207C144 + 0,301C166 + 0,030C123 -0,534C456	0,017
[0,891, 0,454, 0,000]	[0,928, 0,372, 0,000]	0,453	0,571C111 + 0,417C112 + 0,000C144 + 1,692C166 + 0,000C123 + 0,000C456	1,354
[0,891, 0,454, 0,000]	[-0,372, 0,928, 0,000]	0,160	0,039C111 -0,038C112 + 0,000C144 + 0,118C166 + 0,000C123 + 0,000C456	0,043
[0,805, 0,585, 0,105]	[0,841, 0,535, 0,085]	0,437	0,340C111 + 0,642C112 + 0,068C144 + 2,582C166 + 0,011C123 + 0,091C456	1,307
[0,805, 0,585, 0,105]	[-0,539, 0,842, 0,034]	0,175	0,038C111 -0,033C112 -0,013C144 + 0,039C166 -0,005C123 -0,007C456	0,033
[0,805, 0,585, 0,105]	[-0,053,-0,074, 0,996]	0,128	0,001C111 -0,002C112 -0,122C144 + 0,176C166 + 0,001C123 -0,249C456	0,007
[0,694, 0,694, 0,188]	[0,698, 0,698, 0,158]	0,428	0,228C111 + 0,729C112 + 0,253C144 + 2,916C166 + 0,042C123 + 0,338C456	1,284
[0,694, 0,694, 0,188]	[-0,112,-0,112, 0,987]	0,131	0,005C111 -0,012C112 -0,192C144 + 0,276C166 + 0,007C123 -0,411C456	0,012
[0,809, 0,588, 0,000]	[0,844, 0,536, 0,000]	0,438	0,350C111 + 0,644C112 + 0,000C144 + 2,590C166 + 0,000C123 + 0,000C456	1,311
[0,809, 0,588, 0,000]	[-0,536, 0,844, 0,000]	0,175	0,040C111 -0,040C112 + 0,000C144 + 0,025C166 + 0,000C123 + 0,000C456	0,033
[0,705, 0,705, 0,084]	[0,708, 0,705, 0,069]	0,431	0,246C111 + 0,745C112 + 0,052C144 + 2,982C166 + 0,009C123 + 0,069C456	1,292
[0,705, 0,705, 0,084]	[-0,049,-0,049, 0,998]	0,127	0,001C11. -0,001C112 -0,100C144 + 0,144C166 + 0,001C123 -0,202C456	0,006
[0,707, 0,707, 0,000]	[0,707, 0,707, 0,000]	0,431	0,250C111 + 0,750C112 + 0,000C144 + 3,000C166 + 0,000C123 + 0,000C456	1,294

Table 7. Energy Flux Direction for Copper. Values of the second order constants used here are

$C_{11} = 1.684 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.754 \times 10^{12}$ dyn/cm^2, $C_{12} = 1.214 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	Energy Flux Direction	$\mu \times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	1.684
[1.000, 0.000, 0.000]	[0.000, 1.000, 0.000]	[1.000, 0.000, 0.000]	0.754
[1.000, 0.000, 0.000]	[0.000, 0.000, 1.000]	[1.000, 0.000, 0.000]	0.754
[0.976, 0.155, 0.155]	[0.921, 0.275, 0.275]	[0.879, 0.337, 0.337]	1.817
[0.976, 0.155, 0.155]	[-0.389, 0.651, 0.651]	[0.943,-0.236,-0.236]	0.646
[0.976, 0.155, 0.155]	[0.000,-0.707, 0.707]	[0.998, 0.049, 0.049]	0.729
[0.909, 0.295, 0.295]	[0.814, 0.410, 0.410]	[0.768, 0.453, 0.453]	2.054
[0.909, 0.295, 0.295]	[-0.580, 0.576, 0.576]	[0.976,-0.153,-0.153]	0.474
[0.909, 0.295, 0.295]	[0.000,-0.707, 0.707]	[0.990, 0.100, 0.100]	0.664
[0.811, 0.413, 0.413]	[0.729, 0.484, 0.484]	[0.697, 0.507, 0.507]	2.243
[0.811, 0.413, 0.413]	[-0.685, 0.515, 0.515]	[0.972, 0.165, 0.165]	0.372
[0.811, 0.413, 0.413]	[0.000,-0.707, 0.707]	[0.976, 0.155, 0.155]	0.577
[0.697, 0.507, 0.507]	[0.653, 0.535, 0.535]	[0.637, 0.545, 0.545]	2.347
[0.697, 0.507, 0.507]	[-0.757, 0.462, 0.462]	[0.549, 0.591, 0.591]	0.358
[0.697, 0.507, 0.507]	[0.000,-0.707, 0.707]	[0.952, 0.216, 0.216]	0.487
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	2.376
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	[0.075, 0.705, 0.705]	0.408
[0.577, 0.577, 0.577]	[0.000,-0.707, 0.707]	[0.915, 0.285, 0.285]	0.408
[0.988, 0.156, 0.000]	[0.955, 0.297, 0.000]	[0.926, 0.378, 0.000]	1.756
[0.988, 0.156, 0.000]	[-0.297, 0.955, 0.000]	[0.926,-0.376, 0.000]	0.682
[0.988, 0.156, 0.000]	[0.000, 0.000, 1.000]	[0.988, 0.156, 0.000]	0.754
[0.941, 0.306, 0.144]	[0.860, 0.457, 0.229]	[0.813, 0.517, 0.268]	1.950
[0.941, 0.306, 0.144]	[-0.506, 0.826, 0.250]	[0.912,-0.409, 0.010]	0.520
[0.941, 0.306, 0.144]	[-0.074,-0.331, 0.941]	[0.949, 0.293,-0.120]	0.722
[0.858, 0.437, 0.268]	[0.770, 0.531, 0.353]	[0.733, 0.560, 0.387]	2.156
[0.858, 0.437, 0.268]	[-0.626, 0.735, 0.261]	[0.944,-0.251, 0.213]	0.384
[0.858, 0.437, 0.268]	[-0.120,-0.422, 0.899]	[0.903, 0.403,-0.149]	0.652
[0.752, 0.547, 0.367]	[0.693, 0.579, 0.429]	[0.671, 0.587, 0.453]	2.293
[0.752, 0.547, 0.367]	[-0.696, 0.693, 0.190]	[0.775, 0.099, 0.624]	0.327
[0.752, 0.547, 0.367]	[-0.187,-0.430, 0.883]	[0.836, 0.524,-0.164]	0.572
[0.634, 0.634, 0.444]	[0.619, 0.619, 0.485]	[0.612, 0.612, 0.501]	2.351
[0.634, 0.634, 0.444]	[-0.707, 0.707, 0.000]	[0.376, 0.376, 0.847]	0.337
[0.634, 0.634, 0.444]	[-0.343,-0.343, 0.875]	[0.698, 0.698,-0.156]	0.504
[0.951, 0.309, 0.000]	[0.879, 0.477, 0.000]	[0.837, 0.547, 0.000]	1.909
[0.951, 0.309, 0.000]	[-0.477, 0.879, 0.000]	[0.896,-0.445, 0.000]	0.529
[0.951, 0.309, 0.000]	[0.000, 0.000, 1.000]	[0.951, 0.309, 0.000]	0.754
[0.884, 0.450, 0.126]	[0.803, 0.568, 0.182]	[0.767, 0.607, 0.209]	2.085
[0.884, 0.450, 0.126]	[-0.590, 0.801, 0.103]	[0.931,-0.347, 0.114]	0.380
[0.884, 0.450, 0.126]	[-0.087,-0.190, 0.978]	[0.883, 0.447,-0.140]	0.727
[0.787, 0.572, 0.230]	[0.729, 0.618, 0.294]	[0.706, 0.630, 0.324]	2.226
[0.787, 0.572, 0.230]	[-0.665, 0.742, 0.088]	[0.905,-0.029, 0.425]	0.294
[0.787, 0.572, 0.230]	[-0.164,-0.260, 0.952]	[0.796, 0.568,-0.207]	0.671
[0.672, 0.672, 0.311]	[0.657, 0.657, 0.371]	[0.648, 0.648, 0.399]	2.296
[0.672, 0.672, 0.311]	[-0.707, 0.707, 0.000]	[0.488, 0.488, 0.724]	0.285
[0.672, 0.672, 0.311]	[-0.263,-0.263, 0.928]	[0.689, 0.689,-0.227]	0.611
[0.891, 0.454, 0.000]	[0.814, 0.581, 0.000]	[0.781, 0.625, 0.000]	2.061
[0.891, 0.454, 0.000]	[-0.581, 0.814, 0.000]	[0.931,-0.365, 0.000]	0.377
[0.891, 0.454, 0.000]	[0.000, 0.000, 1.000]	[0.891, 0.454, 0.000]	0.754
[0.805, 0.585, 0.105]	[0.752, 0.644, 0.143]	[0.733, 0.661, 0.163]	2.180
[0.805, 0.585, 0.105]	[-0.654, 0.756, 0.036]	[0.977,-0.071, 0.203]	0.277
[0.805, 0.585, 0.105]	[-0.085,-0.120, 0.989]	[0.803, 0.583,-0.127]	0.735
[0.694, 0.694, 0.188]	[0.686, 0.686, 0.242]	[0.681, 0.681, 0.270]	2.243
[0.694, 0.694, 0.188]	[-0.707, 0.707, 0.000]	[0.602, 0.602, 0.524]	0.253
[0.694, 0.694, 0.188]	[-0.171,-0.171, 0.970]	[0.693, 0.693,-0.197]	0.696
[0.809, 0.588, 0.000]	[0.759, 0.651, 0.000]	[0.741, 0.671, 0.000]	2.166
[0.809, 0.588, 0.000]	[-0.651, 0.759, 0.000]	[0.997,-0.080, 0.000]	0.272
[0.809, 0.588, 0.000]	[0.000, 0.000, 1.000]	[0.809, 0.588, 0.000]	0.754
[0.705, 0.705, 0.084]	[0.703, 0.703, 0.113]	[0.701, 0.701, 0.128]	2.211
[0.705, 0.705, 0.084]	[-0.707, 0.707, 0.000]	[0.683, 0.683, 0.261]	0.239
[0.705, 0.705, 0.084]	[-0.080,-0.080, 0.994]	[0.703, 0.703,-0.105]	0.742
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	2.203
[0.707, 0.707, 0.000]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	0.235
[0.707, 0.707, 0.000]	[0.000, 0.000, 1.000]	[0.707, 0.707, 0.000]	0.754

Table 8. Energy Flux Direction for Gold. Values of the second order constants used here are

$C_{11} = 1.86 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.420 \times 10^{12}$ dyn/cm^2, $C_{12} = 1.57 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	Energy Flux Direction	$\mu \times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	1.860
[1.000, 0.000, 0.000]	[0.000, 1.000, 0.000]	[1.000, 0.000, 0.000]	0.420
[1.000, 0.000, 0.000]	[0.000, 0.000, 1.000]	[1.000, 0.000, 0.000]	0.420
[0.976, 0.155, 0.155]	[0.958, 0.203, 0.203]	[0.941, 0.240, 0.240]	1.918
[0.976, 0.155, 0.155]	[-0.287, 0.677, 0.677]	[0.972,-0.166,-0.166]	0.375
[0.976, 0.155, 0.155]	[0.000,-0.707, 0.707]	[0.997, 0.055, 0.055]	0.407
[0.909, 0.295, 0.295]	[0.868, 0.351, 0.351]	[0.837, 0.387, 0.387]	2.040
[0.909, 0.295, 0.295]	[-0.496, 0.614, 0.614]	[0.983,-0.128,-0.128]	0.288
[0.909, 0.295, 0.295]	[0.000,-0.707, 0.707]	[0.988, 0.111, 0.111]	0.372
[0.811, 0.413, 0.413]	[0.771, 0.451, 0.451]	[0.743, 0.473, 0.473]	2.148
[0.811, 0.413, 0.413]	[-0.637, 0.545, 0.545]	[0.981, 0.138, 0.138]	0.226
[0.811, 0.413, 0.413]	[0.000,-0.707, 0.707]	[0.970, 0.171, 0.171]	0.326
[0.697, 0.507, 0.507]	[0.674, 0.522, 0.522]	[0.660, 0.531, 0.531]	2.209
[0.697, 0.507, 0.507]	[-0.738, 0.477, 0.477]	[0.611, 0.560, 0.560]	0.212
[0.697, 0.507, 0.507]	[0.000,-0.707, 0.707]	[0.942, 0.236, 0.236]	0.279
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	2.227
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	[0.114, 0.702, 0.702]	0.237
[0.577, 0.577, 0.577]	[0.000,-0.707, 0.707]	[0.899, 0.310, 0.310]	0.237
[0.988, 0.156, 0.000]	[0.978, 0.209, 0.000]	[0.968, 0.252, 0.000]	1.891
[0.988, 0.156, 0.000]	[-0.209, 0.978, 0.000]	[0.959,-0.282, 0.000]	0.389
[0.988, 0.156, 0.000]	[0.000, 0.000, 1.000]	[0.988, 0.156, 0.000]	0.420
[0.941, 0.306, 0.144]	[0.909, 0.375, 0.181]	[0.882, 0.423, 0.208]	1.985
[0.941, 0.306, 0.144]	[-0.411, 0.878, 0.244]	[0.931,-0.363, 0.038]	0.311
[0.941, 0.306, 0.144]	[-0.068,-0.296, 0.953]	[0.949, 0.297,-0.105]	0.403
[0.858, 0.437, 0.268]	[0.817, 0.486, 0.309]	[0.788, 0.516, 0.336]	2.099
[0.858, 0.437, 0.268]	[-0.565, 0.782, 0.264]	[0.946,-0.247, 0.208]	0.234
[0.858, 0.437, 0.268]	[-0.113,-0.390, 0.914]	[0.901, 0.414,-0.133]	0.367
[0.752, 0.547, 0.367]	[0.722, 0.565, 0.398]	[0.703, 0.575, 0.418]	2.179
[0.752, 0.547, 0.367]	[-0.668, 0.719, 0.192]	[0.809, 0.080, 0.582]	0.196
[0.752, 0.547, 0.367]	[-0.178,-0.405, 0.897]	[0.832, 0.536,-0.144]	0.325
[0.634, 0.634, 0.444]	[0.626, 0.626, 0.465]	[0.621, 0.621, 0.478]	2.212
[0.634, 0.634, 0.444]	[-0.707, 0.707, 0.000]	[0.404, 0.404, 0.821]	0.199
[0.634, 0.634, 0.444]	[-0.329,-0.329, 0.885]	[0.701, 0.701,-0.132]	0.288
[0.951, 0.309, 0.000]	[0.923, 0.384, 0.000]	[0.900, 0.436, 0.000]	1.965
[0.951, 0.309, 0.000]	[-0.384, 0.923, 0.000]	[0.922,-0.388, 0.000]	0.315
[0.951, 0.309, 0.000]	[0.000, 0.000, 1.000]	[0.951, 0.309, 0.000]	0.420
[0.884, 0.450, 0.126]	[0.847, 0.510, 0.152]	[0.820, 0.547, 0.170]	2.062
[0.884, 0.450, 0.126]	[-0.526, 0.844, 0.101]	[0.938,-0.327, 0.113]	0.232
[0.884, 0.450, 0.126]	[-0.077,-0.165, 0.983]	[0.885, 0.449,-0.118]	0.407
[0.787, 0.572, 0.230]	[0.758, 0.598, 0.261]	[0.739, 0.612, 0.282]	2.143
[0.787, 0.572, 0.230]	[-0.635, 0.767, 0.088]	[0.920,-0.032, 0.391]	0.180
[0.787, 0.572, 0.230]	[-0.147,-0.232, 0.961]	[0.799, 0.573,-0.180]	0.378
[0.672, 0.672, 0.311]	[0.665, 0.665, 0.340]	[0.660, 0.660, 0.360]	2.182
[0.672, 0.672, 0.311]	[-0.707, 0.707, 0.000]	[0.514, 0.514, 0.687]	0.172
[0.672, 0.672, 0.311]	[-0.241,-0.241, 0.940]	[0.693, 0.693,-0.199]	0.346
[0.891, 0.454, 0.000]	[0.856, 0.517, 0.000]	[0.830, 0.557, 0.000]	2.049
[0.891, 0.454, 0.000]	[-0.517, 0.856, 0.000]	[0.940,-0.341, 0.000]	0.231
[0.891, 0.454, 0.000]	[0.000, 0.000, 1.000]	[0.891, 0.454, 0.000]	0.420
[0.805, 0.585, 0.105]	[0.778, 0.616, 0.122]	[0.761, 0.634, 0.135]	2.119
[0.805, 0.585, 0.105]	[-0.624, 0.781, 0.036]	[0.980,-0.068, 0.185]	0.170
[0.805, 0.585, 0.105]	[-0.074,-0.104, 0.992]	[0.805, 0.584,-0.105]	0.411
[0.694, 0.694, 0.188]	[0.691, 0.691, 0.213]	[0.688, 0.688, 0.231]	2.155
[0.694, 0.694, 0.188]	[-0.707, 0.707, 0.000]	[0.618, 0.618, 0.485]	0.155
[0.694, 0.694, 0.188]	[-0.151,-0.151, 0.977]	[0.697, 0.697,-0.167]	0.391
[0.809, 0.588, 0.000]	[0.784, 0.621, 0.000]	[0.768, 0.641, 0.000]	2.112
[0.809, 0.588, 0.000]	[-0.621, 0.784, 0.000]	[0.997,-0.076, 0.000]	0.168
[0.809, 0.588, 0.000]	[0.000, 0.000, 1.000]	[0.809, 0.588, 0.000]	0.420
[0.705, 0.705, 0.084]	[0.704, 0.704, 0.097]	[0.703, 0.703, 0.106]	2.139
[0.705, 0.705, 0.084]	[-0.707, 0.707, 0.000]	[0.687, 0.687, 0.237]	0.147
[0.705, 0.705, 0.084]	[-0.069,-0.069, 0.995]	[0.704, 0.704,-0.087]	0.414
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	2.135
[0.707, 0.707, 0.000]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	0.145
[0.707, 0.707, 0.000]	[0.000, 0.000, 1.000]	[0.707, 0.707, 0.000]	0.420

Table 9. Energy Flux Direction for Germanium. Values of the second order constants used here are

$C_{11} = 1.289 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.671 \times 10^{12}$ dyn/cm^2, $C_{12} = 0.483 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	Energy Flux Direction	$\mu \times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	1.289
[1.000, 0.000, 0.000]	[0.000, 1.000, 0.000]	[1.000, 0.000, 0.000]	0.671
[1.000, 0.000, 0.000]	[0.000, 0.000, 1.000]	[1.000, 0.000, 0.000]	0.671
[0.976, 0.155, 0.155]	[0.933, 0.254, 0.254]	[0.917, 0.281, 0.281]	1.354
[0.976, 0.155, 0.155]	[-0.359, 0.660, 0.660]	[0.996,-0.067,-0.067]	0.619
[0.976, 0.155, 0.155]	[0.000,-0.707, 0.707]	[0.991, 0.094, 0.094]	0.658
[0.909, 0.295, 0.295]	[0.830, 0.395, 0.395]	[0.810, 0.414, 0.414]	1.476
[0.909, 0.295, 0.295]	[-0.558, 0.587, 0.587]	[0.996, 0.062, 0.062]	0.531
[0.909, 0.295, 0.295]	[0.000,-0.707, 0.707]	[0.964, 0.188, 0.188]	0.624
[0.811, 0.413, 0.413]	[0.740, 0.476, 0.476]	[0.726, 0.486, 0.486]	1.576
[0.811, 0.413, 0.413]	[-0.673, 0.523, 0.523]	[0.901, 0.307, 0.307]	0.476
[0.811, 0.413, 0.413]	[0.000,-0.707, 0.707]	[0.918, 0.281, 0.281]	0.579
[0.697, 0.507, 0.507]	[0.659, 0.532, 0.532]	[0.652, 0.536, 0.536]	1.631
[0.697, 0.507, 0.507]	[-0.753, 0.466, 0.466]	[0.646, 0.540, 0.540]	0.467
[0.697, 0.507, 0.507]	[0.000,-0.707, 0.707]	[0.851, 0.371, 0.371]	0.533
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	1.646
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	[0.356, 0.661, 0.661]	0.492
[0.577, 0.577, 0.577]	[0.000,-0.707, 0.707]	[0.762, 0.458, 0.458]	0.492
[0.988, 0.156, 0.000]	[0.963, 0.269, 0.000]	[0.953, 0.304, 0.000]	1.324
[0.988, 0.156, 0.000]	[-0.269, 0.963, 0.000]	[0.989,-0.151, 0.000]	0.636
[0.988, 0.156, 0.000]	[0.000, 0.000, 1.000]	[0.988, 0.156, 0.000]	0.671
[0.941, 0.306, 0.144]	[0.874, 0.435, 0.215]	[0.856, 0.461, 0.233]	1.422
[0.941, 0.306, 0.144]	[-0.480, 0.841, 0.250]	[0.991,-0.106, 0.076]	0.555
[0.941, 0.306, 0.144]	[-0.073,-0.321, 0.944]	[0.953, 0.301,-0.008]	0.654
[0.858, 0.437, 0.268]	[0.783, 0.520, 0.341]	[0.768, 0.532, 0.357]	1.530
[0.858, 0.437, 0.268]	[-0.611, 0.747, 0.262]	[0.961, 0.103, 0.255]	0.482
[0.858, 0.437, 0.268]	[-0.119,-0.413, 0.903]	[0.903, 0.429, 0.031]	0.619
[0.752, 0.547, 0.367]	[0.701, 0.576, 0.421]	[0.691, 0.579, 0.432]	1.603
[0.752, 0.547, 0.367]	[-0.689, 0.699, 0.190]	[0.792, 0.368, 0.487]	0.451
[0.752, 0.547, 0.367]	[-0.185,-0.423, 0.887]	[0.828, 0.556, 0.076]	0.577
[0.634, 0.634, 0.444]	[0.620, 0.620, 0.480]	[0.618, 0.618, 0.487]	1.633
[0.634, 0.634, 0.444]	[-0.707, 0.707, 0.000]	[0.545, 0.545, 0.637]	0.456
[0.634, 0.634, 0.444]	[-0.339,-0.339, 0.877]	[0.701, 0.701, 0.130]	0.542
[0.951, 0.309, 0.000]	[0.893, 0.451, 0.000]	[0.876, 0.482, 0.000]	1.401
[0.951, 0.309, 0.000]	[-0.451, 0.893, 0.000]	[0.991,-0.133, 0.000]	0.559
[0.951, 0.309, 0.000]	[0.000, 0.000, 1.000]	[0.951, 0.309, 0.000]	0.671
[0.884, 0.450, 0.126]	[0.815, 0.553, 0.174]	[0.801, 0.570, 0.186]	1.493
[0.884, 0.450, 0.126]	[-0.574, 0.813, 0.102]	[0.991, 0.043, 0.130]	0.480
[0.884, 0.450, 0.126]	[-0.084,-0.183, 0.979]	[0.891, 0.453,-0.027]	0.657
[0.787, 0.572, 0.230]	[0.736, 0.613, 0.285]	[0.727, 0.618, 0.300]	1.568
[0.787, 0.572, 0.230]	[-0.657, 0.748, 0.088]	[0.884, 0.338, 0.324]	0.434
[0.787, 0.572, 0.230]	[-0.159,-0.253, 0.954]	[0.812, 0.584,-0.022]	0.629
[0.672, 0.672, 0.311]	[0.659, 0.659, 0.363]	[0.655, 0.655, 0.376]	1.604
[0.672, 0.672, 0.311]	[-0.707, 0.707, 0.000]	[0.621, 0.621, 0.478]	0.429
[0.672, 0.672, 0.311]	[-0.257,-0.257, 0.932]	[0.707, 0.707, 0.006]	0.598
[0.891, 0.454, 0.000]	[0.825, 0.565, 0.000]	[0.813, 0.583, 0.000]	1.481
[0.891, 0.454, 0.000]	[-0.565, 0.825, 0.000]	[1.000, 0.031, 0.000]	0.479
[0.891, 0.454, 0.000]	[0.000, 0.000, 1.000]	[0.891, 0.454, 0.000]	0.671
[0.805, 0.585, 0.105]	[0.759, 0.637, 0.137]	[0.751, 0.644, 0.147]	1.544
[0.805, 0.585, 0.105]	[-0.646, 0.762, 0.036]	[0.930, 0.334, 0.152]	0.425
[0.805, 0.585, 0.105]	[-0.082,-0.116, 0.990]	[0.809, 0.587,-0.028]	0.661
[0.694, 0.694, 0.188]	[0.687, 0.687, 0.234]	[0.685, 0.685, 0.247]	1.577
[0.694, 0.694, 0.188]	[-0.707, 0.707, 0.000]	[0.674, 0.674, 0.304]	0.412
[0.694, 0.694, 0.188]	[-0.166,-0.166, 0.972]	[0.707, 0.707,-0.034]	0.641
[0.809, 0.588, 0.000]	[0.765, 0.644, 0.000]	[0.759, 0.652, 0.000]	1.537
[0.809, 0.588, 0.000]	[-0.644, 0.765, 0.000]	[0.943, 0.334, 0.000]	0.423
[0.809, 0.588, 0.000]	[0.000, 0.000, 1.000]	[0.809, 0.588, 0.000]	0.671
[0.705, 0.705, 0.084]	[0.703, 0.703, 0.108]	[0.702, 0.702, 0.116]	1.561
[0.705, 0.705, 0.084]	[-0.707, 0.707, 0.000]	[0.700, 0.700, 0.139]	0.405
[0.705, 0.705, 0.084]	[-0.077,-0.077, 0.994]	[0.707, 0.707,-0.024]	0.665
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	1.557
[0.707, 0.707, 0.000]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	0.403
[0.707, 0.707, 0.000]	[0.000, 0.000, 1.000]	[0.707, 0.707, 0.000]	0.671

Table 10. Energy Flux Direction for Silicon. Values of the second order constants used here are

$C_{11} = 1.657 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.796 \times 10^{12}$ dyn/cm^2, $C_{12} = 0.639 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	Energy Flux Direction	$\mu \times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	1.657
[1.000, 0.000, 0.000]	[0.000, 1.000, 0.000]	[1.000, 0.000, 0.000]	0.796
[1.000, 0.000, 0.000]	[0.000, 0.000, 1.000]	[1.000, 0.000, 0.000]	0.796
[0.976, 0.155, 0.155]	[0.944, 0.234, 0.234]	[0.930, 0.259, 0.259]	1.723
[0.976, 0.155, 0.155]	[-0.331, 0.667, 0.667]	[0.999,-0.037,-0.037]	0.743
[0.976, 0.155, 0.155]	[0.000,-0.707, 0.707]	[0.990, 0.100, 0.100]	0.782
[0.909, 0.295, 0.295]	[0.844, 0.379, 0.379]	[0.826, 0.399, 0.399]	1.853
[0.909, 0.295, 0.295]	[-0.536, 0.597, 0.597]	[0.992, 0.087, 0.087]	0.650
[0.909, 0.295, 0.295]	[0.000,-0.707, 0.707]	[0.959, 0.199, 0.199]	0.746
[0.811, 0.413, 0.413]	[0.751, 0.467, 0.467]	[0.737, 0.478, 0.478]	1.962
[0.811, 0.413, 0.413]	[-0.661, 0.531, 0.531]	[0.895, 0.315, 0.315]	0.589
[0.811, 0.413, 0.413]	[0.000,-0.707, 0.707]	[0.908, 0.296, 0.296]	0.698
[0.697, 0.507, 0.507]	[0.664, 0.529, 0.529]	[0.657, 0.533, 0.533]	2.022
[0.697, 0.507, 0.507]	[-0.748, 0.470, 0.470]	[0.657, 0.533, 0.533]	0.578
[0.697, 0.507, 0.507]	[0.000,-0.707, 0.707]	[0.836, 0.388, 0.388]	0.649
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	2.040
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	[0.385, 0.653, 0.653]	0.605
[0.577, 0.577, 0.577]	[0.000,-0.707, 0.707]	[0.742, 0.474, 0.474]	0.605
[0.988, 0.156, 0.000]	[0.969, 0.246, 0.000]	[0.961, 0.276, 0.000]	1.692
[0.988, 0.156, 0.000]	[-0.246, 0.969, 0.000]	[0.994,-0.110, 0.000]	0.761
[0.988, 0.156, 0.000]	[0.000, 0.000, 1.000]	[0.988, 0.156, 0.000]	0.796
[0.941, 0.306, 0.144]	[0.888, 0.413, 0.203]	[0.871, 0.440, 0.219]	1.795
[0.941, 0.306, 0.144]	[-0.455, 0.855, 0.248]	[0.994,-0.062, 0.087]	0.675
[0.941, 0.306, 0.144]	[-0.071,-0.312, 0.947]	[0.953, 0.303, 0.007]	0.778
[0.858, 0.437, 0.268]	[0.795, 0.509, 0.330]	[0.780, 0.522, 0.345]	1.912
[0.858, 0.437, 0.268]	[-0.595, 0.760, 0.263]	[0.957, 0.136, 0.257]	0.597
[0.858, 0.437, 0.268]	[-0.117,-0.405, 0.907]	[0.900, 0.432, 0.055]	0.740
[0.752, 0.547, 0.367]	[0.708, 0.572, 0.413]	[0.699, 0.576, 0.424]	1.992
[0.752, 0.547, 0.367]	[-0.682, 0.706, 0.191]	[0.793, 0.386, 0.471]	0.561
[0.752, 0.547, 0.367]	[-0.182,-0.417, 0.890]	[0.823, 0.558, 0.106]	0.696
[0.634, 0.634, 0.444]	[0.622, 0.622, 0.475]	[0.620, 0.620, 0.482]	2.025
[0.634, 0.634, 0.444]	[-0.707, 0.707, 0.000]	[0.559, 0.559, 0.613]	0.566
[0.634, 0.634, 0.444]	[-0.336,-0.336, 0.880]	[0.698, 0.698, 0.164]	0.658
[0.951, 0.309, 0.000]	[0.905, 0.426, 0.000]	[0.890, 0.457, 0.000]	1.773
[0.951, 0.309, 0.000]	[-0.426, 0.905, 0.000]	[0.996,-0.085, 0.000]	0.680
[0.951, 0.309, 0.000]	[0.000, 0.000, 1.000]	[0.951, 0.309, 0.000]	0.796
[0.884, 0.450, 0.126]	[0.826, 0.538, 0.166]	[0.812, 0.556, 0.177]	1.873
[0.884, 0.450, 0.126]	[-0.557, 0.824, 0.102]	[0.988, 0.085, 0.131]	0.595
[0.884, 0.450, 0.126]	[-0.082,-0.177, 0.981]	[0.891, 0.453,-0.011]	0.782
[0.787, 0.572, 0.230]	[0.744, 0.608, 0.276]	[0.735, 0.614, 0.290]	1.954
[0.787, 0.572, 0.230]	[-0.650, 0.755, 0.088]	[0.878, 0.364, 0.311]	0.544
[0.787, 0.572, 0.230]	[-0.155,-0.245, 0.957]	[0.811, 0.585, 0.004]	0.751
[0.672, 0.672, 0.311]	[0.661, 0.661, 0.355]	[0.658, 0.658, 0.367]	1.994
[0.672, 0.672, 0.311]	[-0.707, 0.707, 0.000]	[0.630, 0.630, 0.455]	0.537
[0.672, 0.672, 0.311]	[-0.251,-0.251, 0.935]	[0.707, 0.707, 0.038]	0.718
[0.891, 0.454, 0.000]	[0.837, 0.548, 0.000]	[0.823, 0.568, 0.000]	1.860
[0.891, 0.454, 0.000]	[-0.548, 0.837, 0.000]	[0.997, 0.076, 0.000]	0.593
[0.891, 0.454, 0.000]	[0.000, 0.000, 1.000]	[0.891, 0.454, 0.000]	0.796
[0.805, 0.585, 0.105]	[0.766, 0.630, 0.132]	[0.758, 0.638, 0.140]	1.929
[0.805, 0.585, 0.105]	[-0.638, 0.769, 0.036]	[0.920, 0.363, 0.146]	0.534
[0.805, 0.585, 0.105]	[-0.079,-0.112, 0.991]	[0.809, 0.588,-0.014]	0.786
[0.694, 0.694, 0.188]	[0.689, 0.689, 0.227]	[0.687, 0.687, 0.239]	1.965
[0.694, 0.694, 0.188]	[-0.707, 0.707, 0.000]	[0.677, 0.677, 0.287]	0.519
[0.694, 0.694, 0.188]	[-0.160,-0.160, 0.974]	[0.707, 0.707,-0.010]	0.765
[0.809, 0.588, 0.000]	[0.772, 0.636, 0.000]	[0.764, 0.645, 0.000]	1.922
[0.809, 0.588, 0.000]	[-0.636, 0.772, 0.000]	[0.932, 0.363, 0.000]	0.531
[0.809, 0.588, 0.000]	[0.000, 0.000, 1.000]	[0.809, 0.588, 0.000]	0.796
[0.705, 0.705, 0.084]	[0.703, 0.703, 0.104]	[0.703, 0.703, 0.111]	1.948
[0.705, 0.705, 0.084]	[-0.707, 0.707, 0.000]	[0.701, 0.701, 0.131]	0.511
[0.705, 0.705, 0.084]	[-0.074,-0.074, 0.995]	[0.707, 0.707,-0.012]	0.789
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	1.944
[0.707, 0.707, 0.000]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	0.509
[0.707, 0.707, 0.000]	[0.000, 0.000, 1.000]	[0.707, 0.707, 0.000]	0.796

Table 11. Energy Flux Direction for Potassium Chloride. Values of the second order constants used here are

$C_{11} = 0.398 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.00625 \times 10^{12}$ dyn/cm^2, $C_{12} = 0.062 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	Energy Flux Direction	$\mu \times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	0.398
[1.000, 0.000, 0.000]	[0.000, 1.000, 0.000]	[1.000, 0.000, 0.000]	0.006
[1.000, 0.000, 0.000]	[0.000, 0.000, 1.000]	[1.000, 0.000, 0.000]	0.006
[0.976, 0.155, 0.155]	[0.999, 0.028, 0.028]	[1.000, 0.007, 0.007]	0.380
[0.976, 0.155, 0.155]	[-0.040, 0.707, 0.707]	[0.124, 0.702, 0.702]	0.017
[0.976, 0.155, 0.155]	[0.000,-0.707, 0.707]	[0.164, 0.698, 0.698]	0.014
[0.909, 0.295, 0.295]	[0.996, 0.064, 0.064]	[1.000, 0.018, 0.018]	0.332
[0.909, 0.295, 0.295]	[-0.090, 0.704, 0.704]	[0.065, 0.706, 0.706]	0.044
[0.909, 0.295, 0.295]	[0.000,-0.707, 0.707]	[0.081, 0.705, 0.705]	0.034
[0.811, 0.413, 0.413]	[0.985, 0.122, 0.122]	[0.999, 0.038, 0.038]	0.270
[0.811, 0.413, 0.413]	[-0.172, 0.697, 0.697]	[0.062, 0.706, 0.706]	0.079
[0.811, 0.413, 0.413]	[0.000,-0.707, 0.707]	[0.052, 0.706, 0.706]	0.062
[0.697, 0.507, 0.507]	[0.929, 0.261, 0.261]	[0.986, 0.117, 0.117]	0.210
[0.697, 0.507, 0.507]	[-0.369, 0.657, 0.657]	[0.186, 0.695, 0.695]	0.111
[0.697, 0.507, 0.507]	[0.000,-0.707, 0.707]	[0.036, 0.707, 0.707]	0.089
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	0.182
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	[0.934, 0.253, 0.253]	0.114
[0.577, 0.577, 0.577]	[0.000,-0.707, 0.707]	[0.026, 0.707, 0.707]	0.114
[0.988, 0.156, 0.000]	[1.000, 0.028, 0.000]	[1.000, 0.007, 0.000]	0.389
[0.988, 0.156, 0.000]	[-0.028, 1.000, 0.000]	[0.102, 0.995, 0.000]	0.016
[0.988, 0.156, 0.000]	[0.000, 0.000, 1.000]	[0.988, 0.156, 0.000]	0.006
[0.941, 0.306, 0.144]	[0.998, 0.063, 0.028]	[1.000, 0.017, 0.007]	0.355
[0.941, 0.306, 0.144]	[-0.065, 0.994, 0.087]	[0.052, 0.998, 0.024]	0.042
[0.941, 0.306, 0.144]	[-0.022,-0.088, 0.996]	[0.109, 0.039, 0.993]	0.014
[0.858, 0.437, 0.268]	[0.991, 0.119, 0.062]	[0.999, 0.036, 0.017]	0.299
[0.858, 0.437, 0.268]	[-0.126, 0.983, 0.132]	[0.041, 0.998, 0.039]	0.079
[0.858, 0.437, 0.268]	[-0.046,-0.138, 0.989]	[0.056, 0.040, 0.998]	0.032
[0.752, 0.547, 0.367]	[0.961, 0.250, 0.121]	[0.994, 0.103, 0.040]	0.238
[0.752, 0.547, 0.367]	[-0.266, 0.954, 0.138]	[0.080, 0.996, 0.043]	0.117
[0.752, 0.547, 0.367]	[-0.081,-0.165, 0.983]	[0.039, 0.045, 0.998]	0.055
[0.634, 0.634, 0.444]	[0.688, 0.688, 0.232]	[0.702, 0.702, 0.124]	0.197
[0.634, 0.634, 0.444]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.018]	0.136
[0.634, 0.634, 0.444]	[-0.164,-0.164, 0.973]	[0.045, 0.045, 0.998]	0.077
[0.951, 0.309, 0.000]	[0.998, 0.063, 0.000]	[1.000, 0.017, 0.000]	0.362
[0.951, 0.309, 0.000]	[-0.063, 0.998, 0.000]	[0.051, 0.999, 0.000]	0.042
[0.951, 0.309, 0.000]	[0.000, 0.000, 1.000]	[0.951, 0.309, 0.000]	0.006
[0.884, 0.450, 0.126]	[0.993, 0.118, 0.026]	[0.999, 0.035, 0.007]	0.316
[0.884, 0.450, 0.126]	[-0.119, 0.992, 0.042]	[0.040, 0.999, 0.011]	0.083
[0.884, 0.450, 0.126]	[-0.021,-0.045, 0.999]	[0.116, 0.059, 0.991]	0.012
[0.787, 0.572, 0.230]	[0.967, 0.246, 0.061]	[0.995, 0.099, 0.018]	0.258
[0.787, 0.572, 0.230]	[-0.249, 0.967, 0.056]	[0.072, 0.997, 0.015]	0.127
[0.787, 0.572, 0.230]	[-0.046,-0.069, 0.997]	[0.058, 0.044, 0.997]	0.026
[0.672, 0.672, 0.311]	[0.702, 0.702, 0.116]	[0.706, 0.706, 0.049]	0.216
[0.672, 0.672, 0.311]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.012]	0.152
[0.672, 0.672, 0.311]	[-0.082,-0.082, 0.993]	[0.040, 0.040, 0.998]	0.042
[0.891, 0.454, 0.000]	[0.993, 0.117, 0.000]	[0.999, 0.035, 0.000]	0.321
[0.891, 0.454, 0.000]	[-0.117, 0.993, 0.000]	[0.040, 0.999, 0.000]	0.084
[0.891, 0.454, 0.000]	[0.000, 0.000, 1.000]	[0.891, 0.454, 0.000]	0.006
[0.805, 0.585, 0.105]	[0.969, 0.244, 0.026]	[0.995, 0.097, 0.007]	0.268
[0.805, 0.585, 0.105]	[-0.245, 0.969, 0.022]	[0.070, 0.998, 0.006]	0.132
[0.805, 0.585, 0.105]	[-0.020,-0.027, 0.999]	[0.126, 0.091, 0.988]	0.010
[0.694, 0.694, 0.188]	[0.706, 0.706, 0.060]	[0.707, 0.707, 0.024]	0.229
[0.694, 0.694, 0.188]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.007]	0.162
[0.694, 0.694, 0.188]	[-0.043,-0.043, 0.998]	[0.062, 0.062, 0.996]	0.019
[0.809, 0.588, 0.000]	[0.970, 0.244, 0.000]	[0.995, 0.097, 0.000]	0.271
[0.809, 0.588, 0.000]	[-0.244, 0.970, 0.000]	[0.069, 0.998, 0.000]	0.133
[0.809, 0.588, 0.000]	[0.000, 0.000, 1.000]	[0.809, 0.588, 0.000]	0.006
[0.705, 0.705, 0.084]	[0.707, 0.707, 0.025]	[0.707, 0.707, 0.010]	0.235
[0.705, 0.705, 0.084]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.003]	0.167
[0.705, 0.705, 0.084]	[-0.018,-0.018, 1.000]	[0.137, 0.137, 0.981]	0.009
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	0.236
[0.707, 0.707, 0.000]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	0.168
[0.707, 0.707, 0.000]	[0.000, 0.000, 1.000]	[0.707, 0.707, 0.000]	0.006

Table 12. Energy Flux Direction for Sodium Chloride. Values of the second order constants used here are

$C_{11} = 0.487 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.126 \times 10^{12}$ dyn/cm^2, $C_{12} = 0.124 \times 10^{12}$ dyn/cm^2.

Propagation Direction	Polarization Direction	Energy Flux Direction	$\mu \times 10^{-12}$ (dyn/cm^2)
[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	[1.000, 0.000, 0.000]	0.487
[1.000, 0.000, 0.000]	[0.000, 1.000, 0.000]	[1.000, 0.000, 0.000]	0.126
[1.000, 0.000, 0.000]	[0.000, 0.000, 1.000]	[1.000, 0.000, 0.000]	0.126
[0.976, 0.155, 0.155]	[0.988, 0.110, 0.110]	[0.990, 0.098, 0.098]	0.478
[0.976, 0.155, 0.155]	[-0.156, 0.698, 0.698]	[0.913, 0.289, 0.289]	0.132
[0.976, 0.155, 0.155]	[0.000,-0.707, 0.707]	[0.952, 0.217, 0.217]	0.129
[0.909, 0.295, 0.295]	[0.946, 0.229, 0.229]	[0.956, 0.208, 0.208]	0.457
[0.909, 0.295, 0.295]	[-0.324, 0.669, 0.669]	[0.769, 0.452, 0.452]	0.147
[0.909, 0.295, 0.295]	[0.000,-0.707, 0.707]	[0.834, 0.390, 0.390]	0.136
[0.811, 0.413, 0.413]	[0.863, 0.357, 0.357]	[0.880, 0.336, 0.336]	0.433
[0.811, 0.413, 0.413]	[-0.505, 0.610, 0.610]	[0.692, 0.511, 0.511]	0.161
[0.811, 0.413, 0.413]	[0.000,-0.707, 0.707]	[0.694, 0.509, 0.509]	0.145
[0.697, 0.507, 0.507]	[0.733, 0.481, 0.481]	[0.747, 0.470, 0.470]	0.418
[0.697, 0.507, 0.507]	[-0.680, 0.518, 0.518]	[0.689, 0.512, 0.512]	0.167
[0.697, 0.507, 0.507]	[0.000,-0.707, 0.707]	[0.560, 0.586, 0.586]	0.155
[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	[0.577, 0.577, 0.577]	0.413
[0.577, 0.577, 0.577]	[-0.816, 0.408, 0.408]	[0.699, 0.505, 0.505]	0.163
[0.577, 0.577, 0.577]	[0.000,-0.707, 0.707]	[0.441, 0.635, 0.635]	0.163
[0.988, 0.156, 0.000]	[0.994, 0.110, 0.000]	[0.995, 0.098, 0.000]	0.482
[0.988, 0.156, 0.000]	[-0.110, 0.994, 0.000]	[0.932, 0.362, 0.000]	0.131
[0.988, 0.156, 0.000]	[0.000, 0.000, 1.000]	[0.988, 0.156, 0.000]	0.126
[0.941, 0.306, 0.144]	[0.967, 0.231, 0.106]	[0.973, 0.208, 0.095]	0.467
[0.941, 0.306, 0.144]	[-0.248, 0.947, 0.205]	[0.792, 0.590, 0.154]	0.143
[0.941, 0.306, 0.144]	[-0.053,-0.225, 0.973]	[0.908, 0.299, 0.295]	0.129
[0.858, 0.437, 0.268]	[0.905, 0.367, 0.215]	[0.919, 0.342, 0.198]	0.444
[0.858, 0.437, 0.268]	[-0.414, 0.875, 0.252]	[0.690, 0.679, 0.250]	0.159
[0.858, 0.437, 0.268]	[-0.096,-0.317, 0.944]	[0.773, 0.410, 0.484]	0.136
[0.752, 0.547, 0.367]	[0.795, 0.513, 0.323]	[0.811, 0.499, 0.307]	0.425
[0.752, 0.547, 0.367]	[-0.586, 0.787, 0.193]	[0.665, 0.686, 0.294]	0.170
[0.752, 0.547, 0.367]	[-0.155,-0.342, 0.927]	[0.636, 0.486, 0.599]	0.145
[0.634, 0.634, 0.444]	[0.644, 0.644, 0.413]	[0.647, 0.647, 0.402]	0.416
[0.634, 0.634, 0.444]	[-0.707, 0.707, 0.000]	[0.669, 0.669, 0.325]	0.171
[0.634, 0.634, 0.444]	[-0.292,-0.292, 0.911]	[0.529, 0.529, 0.664]	0.152
[0.951, 0.309, 0.000]	[0.973, 0.231, 0.000]	[0.978, 0.208, 0.000]	0.470
[0.951, 0.309, 0.000]	[-0.231, 0.973, 0.000]	[0.798, 0.602, 0.000]	0.143
[0.951, 0.309, 0.000]	[0.000, 0.000, 1.000]	[0.951, 0.309, 0.000]	0.126
[0.884, 0.450, 0.126]	[0.924, 0.371, 0.097]	[0.935, 0.343, 0.088]	0.451
[0.884, 0.450, 0.126]	[-0.379, 0.921, 0.090]	[0.693, 0.713, 0.107]	0.160
[0.884, 0.450, 0.126]	[-0.056,-0.120, 0.991]	[0.858, 0.438, 0.269]	0.128
[0.787, 0.572, 0.230]	[0.827, 0.529, 0.191]	[0.841, 0.510, 0.178]	0.432
[0.787, 0.572, 0.230]	[-0.550, 0.830, 0.086]	[0.664, 0.728, 0.172]	0.173
[0.787, 0.572, 0.230]	[-0.113,-0.176, 0.978]	[0.722, 0.527, 0.449]	0.134
[0.672, 0.672, 0.311]	[0.681, 0.681, 0.271]	[0.683, 0.683, 0.258]	0.423
[0.672, 0.672, 0.311]	[-0.707, 0.707, 0.000]	[0.690, 0.690, 0.221]	0.176
[0.672, 0.672, 0.311]	[-0.192,-0.192, 0.963]	[0.587, 0.587, 0.557]	0.140
[0.891, 0.454, 0.000]	[0.928, 0.372, 0.000]	[0.939, 0.343, 0.000]	0.453
[0.891, 0.454, 0.000]	[-0.372, 0.928, 0.000]	[0.695, 0.719, 0.000]	0.160
[0.891, 0.454, 0.000]	[0.000, 0.000, 1.000]	[0.891, 0.454, 0.000]	0.126
[0.805, 0.585, 0.105]	[0.841, 0.535, 0.085]	[0.854, 0.515, 0.079]	0.437
[0.805, 0.585, 0.105]	[-0.539, 0.842, 0.034]	[0.666, 0.742, 0.077]	0.175
[0.805, 0.585, 0.105]	[-0.053,-0.074, 0.996]	[0.788, 0.572, 0.228]	0.128
[0.694, 0.694, 0.188]	[0.698, 0.698, 0.158]	[0.699, 0.699, 0.149]	0.428
[0.694, 0.694, 0.188]	[-0.707, 0.707, 0.000]	[0.701, 0.701, 0.132]	0.180
[0.694, 0.694, 0.188]	[-0.112,-0.112, 0.987]	[0.653, 0.653, 0.385]	0.131
[0.809, 0.588, 0.000]	[0.844, 0.536, 0.000]	[0.857, 0.516, 0.000]	0.438
[0.809, 0.588, 0.000]	[-0.536, 0.844, 0.000]	[0.666, 0.746, 0.000]	0.175
[0.809, 0.588, 0.000]	[0.000, 0.000, 1.000]	[0.809, 0.588, 0.000]	0.126
[0.705, 0.705, 0.084]	[0.705, 0.705, 0.069]	[0.706, 0.706, 0.065]	0.431
[0.705, 0.705, 0.084]	[-0.707, 0.707, 0.000]	[0.706, 0.706, 0.058]	0.181
[0.705, 0.705, 0.084]	[-0.049,-0.049, 0.998]	[0.695, 0.695, 0.185]	0.127
[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	0.431
[0.707, 0.707, 0.000]	[-0.707, 0.707, 0.000]	[0.707, 0.707, 0.000]	0.181
[0.707, 0.707, 0.000]	[0.000, 0.000, 1.000]	[0.707, 0.707, 0.000]	0.126

Table 13. Useful Interactions for Copper. Values of the second order constants used here are:

$C_{11} = 1.684 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.754 \times 10^{12}$ dyn/cm^2, $C_{12} = 1.214 \times 10^{12}$ dyn/cm^2.

Interaction Number 1

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.754 \times 10^{12}$
$\hat{q}^2 = (-0.707, 0.707, 0.000)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 2.203 \times 10^{12}$
$\hat{q}^3 = (0.988, 0.158, 0.000)$, $\hat{P}^3 = (0.954, 0.298, 0.000)$, $\mu_3 = 1.757 \times 10^{12}$
$\omega_2/\omega_1 = 0.333$, $\omega_3/\omega_1 = 1.333$, $G = -0.554C_{166} - 0.468 \times 10^{12}$

Interaction Number 2

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.754 \times 10^{12}$
$\hat{q}^2 = (0.000, 1.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 1.684 \times 10^{12}$
$\hat{q}^3 = (0.799, 0.601, 0.000)$, $\hat{P}^3 = (0.753, 0.657, 0.000)$, $\mu_3 = 2.173 \times 10^{12}$
$\omega_2/\omega_1 = 1.123$, $\omega_3/\omega_1 = 2.124$, $G = +0.978C_{166} + 1.772 \times 10^{12}$

Interaction Number 3

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.754 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.754 \times 10^{12}$
$\hat{q}^3 = (0.387, 0.922, 0.000)$, $\hat{P}^3 = (0.843, -0.538, 0.000)$, $\mu_3 = 0.145 \times 10^{12}$
$\omega_2/\omega_1 = -0.411$, $\omega_3/\omega_1 = 0.589$, $G = -0.351C_{144} + 0.231C_{166} + 0.403C_{456} + 0.266 \times 10^{12}$

Interaction Number 4

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.235 \times 10^{12}$
$\hat{q}^2 = (0.447, -0.894, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.754 \times 10^{12}$
$\hat{q}^3 = (0.928, 0.373, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.754 \times 10^{12}$
$\omega_2/\omega_1 = 0.705$, $\omega_3/\omega_1 = 1.705$, $G = +0.374C_{144} - 0.374C_{166} - 0.176 \times 10^{12}$

Table 13. (Continued)

Interaction Number 5

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.235 \times 10^{12}$
$\hat{q}^2 = (0.707, -0.707, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.754 \times 10^{12}$
$\hat{q}^3 = (0.973, 0.231, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.754 \times 10^{12}$
$\omega_2/\omega_1 = 1.104$, $\omega_3/\omega_1 = 2.104$, $G = +0.426C_{144} - 0.426C_{166} - 0.200 \times 10^{12}$

Interaction Number 6

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (1.000, 0.000, 0.000)$, $\mu_1 = 1.684 \times 10^{12}$
$\hat{q}^2 = (0.577, 0.577, 0.577)$, $\hat{P}^2 = (-0.408, -0.408, 0.816)$, $\mu_2 = 0.408 \times 10^{12}$
$\hat{q}^3 = (0.313, -0.672, -0.672)$, $\hat{P}^3 = (0.000, -0.707, 0.707)$, $\mu_3 = 0.286 \times 10^{12}$
$\omega_2/\omega_1 = -0.581$, $\omega_3/\omega_1 = 0.418$, $G = -0.336C_{112} + 0.154C_{166} + 0.336C_{123} - 0.552 \times 10^{12}$

Interaction Number 7

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.707, 0.707, 0.000)$, $\mu_1 = 2.203 \times 10^{12}$
$\hat{q}^2 = (-0.577, 0.577, 0.577)$, $\hat{P}^2 = (0.707, 0.707, 0.000)$, $\mu_2 = 0.408 \times 10^{12}$
$\hat{q}^3 = (0.911, 0.130, -0.391)$, $\hat{P}^3 = (0.557, -0.144, 0.818)$, $\mu_3 = 0.437 \times 10^{12}$
$\omega_2/\omega_1 = -0.396$, $\omega_3/\omega_1 = 0.605$, $G = -0.107C_{111} + 0.107C_{112} + 0.141C_{144} + 0.141C_{166} + 0.282C_{456} - 0.140 \times 10^{12}$

Interaction Number 8

$\hat{q}^1 = (-0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 2.203 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (1.000, 0.000, 0.000)$, $\mu_2 = 1.684 \times 10^{12}$
$\hat{q}^3 = (-0.865, 0.501, 0.000)$, $\hat{P}^3 = (0.608, 0.794, 0.000)$, $\mu_3 = 0.335 \times 10^{12}$
$\omega_2/\omega_1 = -0.450$, $\omega_3/\omega_1 = 0.550$, $G = -0.263C_{111} + 0.135C_{112} + 0.383C_{166} - 0.855 \times 10^{12}$

Interaction Number 9

$\hat{q}^1 = (-0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 2.203 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.754 \times 10^{12}$
$\hat{q}^3 = (-0.842, 0.539, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.754 \times 10^{12}$
$\omega_2/\omega_1 = -0.233$, $\omega_3/\omega_1 = 0.767$, $G = -0.421C_{144} - 0.421C_{166} - 0.539C_{456} - 1.627 \times 10^{12}$

Table 13. (Continued)

Interaction Number 10

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.754 \times 10^{12}$
$\hat{q}^2 = (-0.577, -0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.408 \times 10^{12}$
$\hat{q}^3 = (0.699, 0.699, -0.154)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.247 \times 10^{12}$
$\omega_2/\omega_1 = -0.256$, $\omega_3/\omega_1 = 0.744$, $G = -0.348C_{144} + 0.348C_{166} + 0.525 \times 10^{12}$

Interaction Number 11

$\hat{q}^1 = (-0.577, -0.577, -0.577)$, $\hat{P}^1 = (0.577, 0.577, 0.577)$, $\mu_1 = 2.376 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 0.754 \times 10^{12}$
$\hat{q}^3 = (-0.811, -0.414, -0.414)$, $\hat{P}^3 = (0.000, -0.707, 0.707)$, $\mu_3 = 0.576 \times 10^{12}$
$\omega_2/\omega_1 = -0.312$, $\omega_3/\omega_1 = 0.687$, $G = +0.004C_{144} - 0.577C_{166} + 0.382C_{456} - 1.080 \times 10^{12}$

Interaction Number 12

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.235 \times 10^{12}$
$\hat{q}^2 = (-0.577, -0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.408 \times 10^{12}$
$\hat{q}^3 = (0.693, 0.693, 0.198)$, $\hat{P}^3 = (-0.180, -0.180, 0.967)$, $\mu_3 = 0.690 \times 10^{12}$
$\omega_2/\omega_1 = 0.359$, $\omega_3/\omega_1 = 1.359$, $G = +0.051C_{111} - 0.129C_{112} - 0.259C_{144} + 0.259C_{166} + 0.078C_{123} + 0.649 \times 10^{12}$

Interaction Number 13

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.754 \times 10^{12}$
$\hat{q}^2 = (-0.577, -0.577, 0.577)$, $\hat{P}^2 = (0.577, 0.577, -0.577)$, $\mu_2 = 2.376 \times 10^{12}$
$\hat{q}^3 = (0.698, 0.698, 0.164)$, $\hat{P}^3 = (0.691, 0.691, 0.213)$, $\mu_3 = 2.234 \times 10^{12}$
$\omega_2/\omega_1 = 0.413$, $\omega_3/\omega_1 = 1.413$, $G = +0.331C_{144} + 0.240C_{166} + 0.662C_{456} + 0.780 \times 10^{12}$

Interaction Number 14

$\hat{q}1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (1.000, 0.000, 0.000)$, $\mu_1 = 1.684 \times 10^{12}$
$\hat{q}^2 = (0.577, 0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.408 \times 10^{12}$
$\hat{q}^3 = (0.313, -0.671, -0.671)$, $\hat{P}^3 = (0.000, -0.707, 0.707)$, $\mu_3 = 0.286 \times 10^{12}$
$\omega_2/\omega_1 = -0.581$, $\omega_3/\omega_1 = 0.418$, $G = +0.194C_{112} - 0.090C_{166} - 0.194C_{123} + 0.318 \times 10^{12}$

Table 13. (Continued)

Interaction Number 15

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\mu_1 = 2.203 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.408 \times 10^{12}$
$\hat{q}^3 = (\ 0.679,\ 0.679,-0.281)$, $\hat{P}^3 = (-0.707,\ 0.707,\ 0.000)$, $\mu_3 = 0.276 \times 10^{12}$
$\omega_2/\omega_1 = -0.372$, $\omega_3/\omega_1 = 0.629$, $G = -0.196C_{111} + 0.196C_{112} - 0.081C_{144} - 0.081C_{166} + 0.162C_{456} - 1.923 \times 10^{12}$

Interaction Number 16

$\hat{q}^1 = (-0.577,-0.577,-0.577)$, $\hat{P}^1 = (\ 0.577,\ 0.577,\ 0.577)$, $\mu_1 = 2.376 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 1.000,\ 0.000)$, $\mu_2 = 0.754 \times 10^{12}$
$\hat{q}^3 = (-0.840,-0.383,-0.383)$, $\hat{P}^3 = (-0.660,\ 0.531,\ 0.531)$, $\mu_3 = 0.391 \times 10^{12}$
$\omega_2/\omega_1 = -0.388$, $\omega_3/\omega_1 = 0.612$, $G = +0.200C_{144} - 0.105C_{166} + 0.400C_{456} + 0.890 \times 10^{12}$

Interaction Number 17

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.754 \times 10^{12}$
$\hat{q}^2 = (\ 0.958,-0.287,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.754 \times 10^{12}$
$\hat{q}^3 = (\ 0.423,\ 0.906,\ 0.000)$, $\hat{P}^3 = (\ 0.827,-0.562,\ 0.000)$, $\mu_3 = 0.408 \times 10^{12}$
$\omega_2/\omega_1 = -0.345$, $\omega_3/\omega_1 = 0.654$, $G = -0.416C_{144} + 0.340C_{166} + 0.243C_{456} + 0.251 \times 10^{12}$

Interaction Number 18

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.754 \times 10^{12}$
$\hat{q}^2 = (\ 0.894,\ 0.447,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.754 \times 10^{12}$
$\hat{q}^3 = (\ 0.323,\ 0.946,\ 0.000)$, $\hat{P}^3 = (\ 0.872,-0.489,\ 0.000)$, $\mu_3 = 0.513 \times 10^{12}$
$\omega_2/\omega_1 = -0.628$, $\omega_3/\omega_1 = 0.372$, $G = -0.204C_{144} + 0.032C_{166} + 0.633C_{456} + 0.284 \times 10^{12}$

Interaction Number 19

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.754 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.408 \times 10^{12}$
$\hat{q}^3 = (\ 0.699,\ 0.699,-0.155)$, $\hat{P}^3 = (-0.707,\ 0.707,\ 0.000)$, $\mu_3 = 0.247 \times 10^{12}$
$\omega_2/\omega_1 = -0.256$, $\omega_3/\omega_1 = 0.744$, $G = -0.348C_{144} + 0.348C_{166} + 0.525 \times 10^{12}$

Table 14. Useful Interactions for Gold. Values of the second order constants used here are:

$C_{11} = 1.86 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.420 \times 10^{12}$ dyn/cm^2, $C_{12} = 1.57 \times 10^{12}$ dyn/cm^2.

Interaction Number 1

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.420 \times 10^{12}$
$\hat{q}^2 = (-0.707, 0.707, 0.000)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 2.135 \times 10^{12}$
$\hat{q}^3 = (0.958, 0.286, 0.000)$, $\hat{P}^3 = (0.933, 0.360, 0.000)$, $\mu_3 = 1.952 \times 10^{12}$
$\omega_2/\omega_1 = 0.733$, $\omega_3/\omega_1 = 1.733$, $G = -0.386C_{166} - 0.317 \times 10^{12}$

Interaction Number 2

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.420 \times 10^{12}$
$\hat{q}^2 = (0.000, 1.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 1.860 \times 10^{12}$
$\hat{q}^3 = (0.648, 0.762, 0.000)$, $\hat{P}^3 = (0.664, 0.747, 0.000)$, $\mu_3 = 2.129 \times 10^{12}$
$\omega_2/\omega_1 = 2.476$, $\omega_3/\omega_1 = 3.476$, $G = +0.990C_{166} + 1.379 \times 10^{12}$

Interaction Number 3

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.420 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.420 \times 10^{12}$
$\hat{q}^3 = (0.406, 0.914, 0.000)$, $\hat{P}^3 = (0.880, -0.476, 0.000)$, $\mu_3 = 0.258 \times 10^{12}$
$\omega_2/\omega_1 = -0.393$, $\omega_3/\omega_1 = 0.606$, $G = -0.307C_{144} + 0.252C_{166} + 0.432C_{456} + 0.168 \times 10^{12}$

Interaction Number 4

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.145 \times 10^{12}$
$\hat{q}^2 = (0.447, -0.894, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.420 \times 10^{12}$
$\hat{q}^3 = (0.915, 0.404, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.420 \times 10^{12}$
$\omega_2/\omega_1 = 0.616$, $\omega_3/\omega_1 = 1.616$, $G = +0.385C_{144} - 0.385C_{166} - 0.112 \times 10^{12}$

Table 14. (Continued)

Interaction Number 5

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.145 \times 10^{12}$
$\hat{q}^2 = (\ 0.707, -0.707,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.420 \times 10^{12}$
$\hat{q}^3 = (\ 0.962,\ 0.274,\ 0.000)$, $\hat{P}^3 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_3 = 0.420 \times 10^{12}$
$\omega_2/\omega_1 = 0.948$, $\omega_3/\omega_1 = 1.948$, $G = +0.437C_{144} - 0.437C_{166} - 0.127 \times 10^{12}$

Interaction Number 6

$\hat{q}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\mu_1 = 1.860 \times 10^{12}$
$\hat{q}^2 = (\ 0.577,\ 0.577,\ 0.577)$, $\hat{P}^2 = (-0.408, -0.408,\ 0.816)$, $\mu_2 = 0.237 \times 10^{12}$
$\hat{q}^3 = (\ 0.009, -0.707, -0.707)$, $\hat{P}^3 = (\ 0.000, -0.707,\ 0.707)$, $\mu_3 = 0.145 \times 10^{12}$
$\omega_2/\omega_1 = -0.610$, $\omega_3/\omega_1 = 0.390$, $G = -0.354C_{112} + 0.005C_{166} + 0.354C_{123} - 1.102 \times 10^{12}$

Interaction Number 7

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\mu_1 = 2.135 \times 10^{12}$
$\hat{q}^2 = (-0.577,\ 0.577,\ 0.577)$, $\hat{P}^2 = (\ 0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.237 \times 10^{12}$
$\hat{q}^3 = (\ 0.884, -0.046, -0.465)$, $\hat{P}^3 = (\ 0.528,\ 0.033,\ 0.849)$, $\mu_3 = 0.224 \times 10^{12}$
$\omega_2/\omega_1 = -0.453$, $\omega_3/\omega_1 = 0.547$, $G = -0.096C_{111} + 0.096C_{112} + 0.092C_{144} + 0.092C_{166} + 0.184C_{456} - 0.497 \times 10^{12}$

Interaction Number 8

$\hat{q}^1 = (-0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 2.135 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\mu_2 = 1.860 \times 10^{12}$
$\hat{q}^3 = (-0.875,\ 0.483,\ 0.000)$, $\hat{P}^3 = (\ 0.541,\ 0.841,\ 0.000)$, $\mu_3 = 0.215 \times 10^{12}$
$\omega_2/\omega_1 = -0.536$, $\omega_3/\omega_1 = 0.464$, $G = -0.237C_{111} + 0.170C_{112} + 0.475C_{166} - 0.586 \times 10^{12}$

Interaction Number 9

$\hat{q}^1 = (-0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 2.135 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.420 \times 10^{12}$
$\hat{q}^3 = (-0.892,\ 0.452,\ 0.000)$, $\hat{P}^3 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_3 = 0.420 \times 10^{12}$
$\omega_2/\omega_1 = -0.306$, $\omega_3/\omega_1 = 0.694$, $G = -0.446C_{144} - 0.446C_{166} - 0.452C_{456} - 1.720 \times 10^{12}$

Table 14. (Continued)

Interaction Number 10

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.420 \times 10^{12}$
$\hat{q}^2 = (-0.577, -0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.237 \times 10^{12}$
$\hat{q}^3 = (0.700, 0.700, -0.144)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.151 \times 10^{12}$
$\omega_2/\omega_1 = -0.238$, $\omega_3/\omega_1 = 0.762$, $G = -0.344C_{144} + 0.344C_{166} + 0.289 \times 10^{12}$

Interaction Number 11

$\hat{q}^1 = (-0.577, -0.577, -0.577)$, $\hat{P}^1 = (0.577, 0.577, 0.577)$, $\mu_1 = 2.227 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 0.420 \times 10^{12}$
$\hat{q}^3 = (-0.864, -0.356, -0.356)$, $\hat{P}^3 = (0.000, -0.707, 0.707)$, $\mu_3 = 0.350 \times 10^{12}$
$\omega_2/\omega_1 = -0.357$, $\omega_3/\omega_1 = 0.642$, $G = -0.036C_{144} - 0.575C_{166} + 0.407C_{456} - 1.159 \times 10^{12}$

Interaction Number 12

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.145 \times 10^{12}$
$\hat{q}^2 = (-0.577, -0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.237 \times 10^{12}$
$\hat{q}^3 = (0.695, 0.695, 0.182)$, $\hat{P}^3 = (-0.146, -0.146, 0.978)$, $\mu_3 = 0.392 \times 10^{12}$
$\omega_2/\omega_1 = 0.325$, $\omega_3/\omega_1 = 1.325$, $G = +0.042C_{111} - 0.114C_{112} - 0.267C_{144} + 0.267C_{166} + 0.073C_{123} + 0.350 \times 10^{12}$

Interaction Number 13

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.420 \times 10^{12}$
$\hat{q}^2 = (-0.577, -0.577, 0.577)$, $\hat{P}^2 = (0.577, 0.577, -0.577)$, $\mu_2 = 2.227 \times 10^{12}$
$\hat{q}^3 = (0.686, 0.686, 0.241)$, $\hat{P}^3 = (0.681, 0.681, 0.269)$, $\mu_3 = 2.166 \times 10^{12}$
$\omega_2/\omega_1 = 0.732$, $\omega_3/\omega_1 = 1.732$, $G = +0.276C_{144} + 0.173C_{166} + 0.553C_{456} + 0.533 \times 10^{12}$

Interaction Number 14

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (1.000, 0.000, 0.000)$, $\mu_1 = 1.860 \times 10^{12}$
$\hat{q}^2 = (0.577, 0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.237 \times 10^{12}$
$\hat{q}^3 = (0.009, -0.707, -0.707)$, $\hat{P}^3 = (0.000, -0.707, 0.707)$, $\mu_3 = 0.145 \times 10^{12}$
$\omega_2/\omega_1 = -0.610$, $\omega_3/\omega_1 = 0.390$, $G = +0.204C_{112} - 0.003C_{166} - 0.204C_{123} + 0.636 \times 10^{12}$

Table 14. (Continued)

Interaction Number 15

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.707, 0.707, 0.000)$, $\mu_1 = 2.135 \times 10^{12}$
$\hat{q}^2 = (-0.577, -0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.237 \times 10^{12}$
$\hat{q}^3 = (0.667, 0.667, -0.330)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.175 \times 10^{12}$
$\omega_2/\omega_1 = -0.400$, $\omega_3/\omega_1 = 0.601$, $G = -0.193C_{111} + 0.193C_{112} - 0.095C_{144} - 095C_{166} + 0.191C_{456} - 1.945 \times 10^{12}$

Interaction Number 16

$\hat{q}^1 = (-0.577, -0.577, -0.577)$, $\hat{P}^1 = (0.577, 0.577, 0.577)$, $\mu_1 = 2.227 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 0.420 \times 10^{12}$
$\hat{q}^3 = (-0.880, -0.335, -0.335)$, $\hat{P}^3 = (-0.547, 0.592, 0.592)$, $\mu_3 = 0.263 \times 10^{12}$
$\omega_2/\omega_1 = -0.408$, $\omega_3/\omega_1 = 0.592$, $G = +0.245C_{144} + 0.037C_{166} + 0.490C_{456} + 1.093 \times 10^{12}$

Interaction Number 17

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.420 \times 10^{12}$
$\hat{q}^2 = (0.958, -0.287, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.420 \times 10^{12}$
$\hat{q}^3 = (0.440, 0.898, 0.000)$, $\hat{P}^3 = (0.863, -0.505\ 0.000)$, $\mu_3 = 0.238 \times 10^{12}$
$\omega_2/\omega_1 = -0.328$, $\omega_3/\omega_1 = 0.672$, $G = -0.385C_{144} + 0.349C_{166} + 0.262C_{456} + 0.156 \times 10^{12}$

Interaction Number 18

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.420 \times 10^{12}$
$\hat{q}^2 = (0.894, 0.447, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.420 \times 10^{12}$
$\hat{q}^3 = (0.343, 0.939, 0.000)$, $\hat{P}^3 = (0.909, -0.418, 0.000)$, $\mu_3 = 0.295 \times 10^{12}$
$\omega_2/\omega_1 = -0.614$, $\omega_3/\omega_1 = 0.386$, $G = -0.149C_{144} + 0.073C_{166} + 0.674C_{456} + 0.184 \times 10^{12}$

Interaction Number 19

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.420 \times 10^{12}$
$\hat{q}^2 = (-0.577, -0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.237 \times 10^{12}$
$\hat{q}^3 = (0.700, 0.700, -0.144)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.151 \times 10^{12}$
$\omega_2/\omega_1 = -0.238$, $\omega_3/\omega_1 = 0.762$, $G = -0.344C_{144} + 0.344C_{166} + 0.289 \times 10^{12}$

Table 15. Useful Interactions for Germanium. Values of the second order constants used here are:

$C_{11} = 1.289 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.671 \times 10^{12}$ dyn/cm^2, $C_{12} = 0.483 \times 10^{12}$ dyn/cm^2.

Interaction Number 1

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.671 \times 10^{12}$
$\hat{q}^2 = (-0.707, 0.707, 0.000)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 1.557 \times 10^{12}$
$\hat{q}^3 = (0.992, 0.129, 0.000)$, $\hat{P}^3 = (0.974, 0.228, 0.000)$, $\mu_3 = 1.313 \times 10^{12}$
$\omega_2/\omega_1 = 0.248$, $\omega_3/\omega_1 = 1.248$, $G = -0.644C_{166} - 0.547 \times 10^{12}$

Interaction Number 2

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.671 \times 10^{12}$
$\hat{q}^2 = (0.000, 1.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 1.289 \times 10^{12}$
$\hat{q}^3 = (0.917, 0.400, 0.000)$, $\hat{P}^3 = (0.850, 0.527, 0.000)$, $\mu_3 = 1.452 \times 10^{12}$
$\omega_2/\omega_1 = 0.605$, $\omega_3/\omega_1 = 1.605$, $G = +0.823C_{166} + 1.109 \times 10^{12}$

Interaction Number 3

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.671 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.671 \times 10^{12}$
$\hat{q}^3 = (0.472, 0.881, 0.000)$, $\hat{P}^3 = (0.817, -0.576, 0.000)$, $\mu_3 = 0.470 \times 10^{12}$
$\omega_2/\omega_1 = -0.328$, $\omega_3/\omega_1 = 0.671$, $G = -0.359C_{144} + 0.273C_{166} + 0.317C_{456} + 0.391 \times 10^{12}$

Interaction Number 4

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.403 \times 10^{12}$
$\hat{q}^2 = (0.447, -0.894, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.671 \times 10^{12}$
$\hat{q}^3 = (0.823, 0.567, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.671 \times 10^{12}$
$\omega_2/\omega_1 = 0.236$, $\omega_3/\omega_1 = 1.236$, $G = +0.438C_{144} - 0.438C_{166} - 0.353 \times 10^{12}$

Table 15. (Continued)

Interaction Number 5

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.403 \times 10^{12}$
$\hat{q}^2 = (\ 0.707, -0.707,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.671 \times 10^{12}$
$\hat{q}^3 = (\ 0.861,\ 0.509,\ 0.000)$, $\hat{P}^3 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_3 = 0.671 \times 10^{12}$
$\omega_2/\omega_1 = 0.332$, $\omega_3/\omega_1 = 1.332$, $G = +0.484c_{144} - 0.484c_{166} - 0.390 \times 10^{12}$

Interaction Number 6

$\hat{q}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\mu_1 = 1.289 \times 10^{12}$
$\hat{q}^2 = (\ 0.577,\ 0.577,\ 0.577)$, $\hat{P}^2 = (-0.408, -0.408,\ 0.816)$, $\mu_2 = 0.492 \times 10^{12}$
$\hat{q}^3 = (\ 0.675, -0.521, -0.521)$, $\hat{P}^3 = (\ 0.000, -0.707,\ 0.707)$, $\mu_3 = 0.525 \times 10^{12}$
$\omega_2/\omega_1 = -0.466$, $\omega_3/\omega_1 = 0.533$, $G = -0.261c_{112} + 0.338c_{166} + 0.261c_{123} + 0.183 \times 10^{12}$

Interaction Number 7

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\mu_1 = 1.557 \times 10^{12}$
$\hat{q}^2 = (-0.577,\ 0.577,\ 0.577)$, $\hat{P}^2 = (\ 0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.492 \times 10^{12}$
$\hat{q}^3 = (\ 0.902,\ 0.319, -0.291)$, $\hat{P}^3 = (-0.569,\ 0.633, -0.524)$, $\mu_3 = 0.524 \times 10^{12}$
$\omega_2/\omega_1 = -0.328$, $\omega_3/\omega_1 = 0.672$, $G = +0.146c_{111} - 0.146c_{112} - 0.135c_{144} - 0.135c_{166} - 0.269c_{456} + 0.037 \times 10^{12}$

Interaction Number 8

$\hat{q}^1 = (-0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 1.557 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\mu_2 = 1.289 \times 10^{12}$
$\hat{q}^3 = (-0.833,\ 0.554,\ 0.000)$, $\hat{P}^3 = (\ 0.625,\ 0.781,\ 0.000)$, $\mu_3 = 0.435 \times 10^{12}$
$\omega_2/\omega_1 = -0.325$, $\omega_3/\omega_1 = 0.675$, $G = -0.260c_{111} + 0.172c_{112} + 0.304c_{166} - 0.717 \times 10^{12}$

Interaction Number 9

$\hat{q}^1 = (-0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 1.557 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.671 \times 10^{12}$
$\hat{q}^3 = (-0.817,\ 0.576,\ 0.000)$, $\hat{P}^3 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_3 = 0.671 \times 10^{12}$
$\omega_2/\omega_1 = -0.195$, $\omega_3/\omega_1 = 0.806$, $G = -0.409c_{144} - 0.409c_{166} - 0.576c_{456} - 1.111 \times 10^{12}$

Table 15. (Continued)

Interaction Number 10

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.671 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.492 \times 10^{12}$
$\hat{q}^3 = (\ 0.705,\ 0.705,-0.076)$, $\hat{P}^3 = (-0.707,\ 0.707,\ 0.000)$, $\mu_3 = 0.405 \times 10^{12}$
$\omega_2/\omega_1 = -0.127$, $\omega_3/\omega_1 = 0.873$, $G = -0.319C_{144} + 0.319C_{166} + 0.428 \times 10^{12}$

Interaction Number 11

$\hat{q}^1 = (-0.577,-0.577,-0.577)$, $\hat{P}^1 = (\ 0.577,\ 0.577,\ 0.577)$, $\mu_1 = 1.646 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 1.000,\ 0.000)$, $\mu_2 = 0.671 \times 10^{12}$
$\hat{q}^3 = (-0.768,-0.453,-0.453)$, $\hat{P}^3 = (\ 0.000,-0.707,\ 0.707)$, $\mu_3 = 0.561 \times 10^{12}$
$\omega_2/\omega_1 = -0.256$, $\omega_3/\omega_1 = 0.744$, $G = +0.033C_{144} - 0.576C_{166} + 0.362C_{456} - 0.695 \times 10^{12}$

Interaction Number 12

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.403 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.492 \times 10^{12}$
$\hat{q}^3 = (\ 0.704,\ 0.704,\ 0.086)$, $\hat{P}^3 = (-0.079,-0.079,\ 0.994)$, $\mu_3 = 0.664 \times 10^{12}$
$\omega_2/\omega_1 = 0.148$, $\omega_3/\omega_1 = 1.148$, $G = +0.023C_{111} - 0.058C_{112} - 0.283C_{144} + 0.283C_{166} + 0.035C_{123} + 0.487 \times 10^{12}$

Interaction Number 13

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.671 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (\ 0.577,\ 0.577,-0.577)$, $\mu_2 = 1.646 \times 10^{12}$
$\hat{q}^3 = (\ 0.701,\ 0.701,\ 0.130)$, $\hat{P}^3 = (\ 0.697,\ 0.697,\ 0.166)$, $\mu_3 = 1.567 \times 10^{12}$
$\omega_2/\omega_1 = 0.300$, $\omega_3/\omega_1 = 1.300$, $G = +0.364C_{144} + 0.286C_{166} + 0.727C_{456} + 0.696 \times 10^{12}$

Interaction Number 14

$\hat{q}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\mu_1 = 1.289 \times 10^{12}$
$\hat{q}^2 = (\ 0.577,\ 0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.492 \times 10^{12}$
$\hat{q}^3 = (\ 0.675,-0.521,-0.521)$, $\hat{P}^3 = (\ 0.000,-0.707,\ 0.707)$, $\mu_3 = 0.525 \times 10^{12}$
$\omega_2/\omega_1 = -0.466$, $\omega_3/\omega_1 = 0.533$, $G = +0.151C_{112} - 0.195C_{166} - 0.151C_{123} - 0.106 \times 10^{12}$

Table 15. (Continued)

Interaction Number 15

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\mu_1 = 1.557 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.492 \times 10^{12}$
$\hat{q}^3 = (\ 0.694,\ 0.694,-0.195)$, $\hat{P}^3 = (-0.707,\ 0.707,\ 0.000)$, $\mu_3 = 0.413 \times 10^{12}$
$\omega_2/\omega_1 = -0.270$, $\omega_3/\omega_1 = 0.731$, $G = -0.200C_{111} + 0.200C_{112} - 0.056C_{144} - 0.056C_{166} + 0.113C_{456} - 1.301 \times 10^{12}$

Interaction Number 16

$\hat{q}^1 = (-0.577,-0.577,-0.577)$, $\hat{P}^1 = (\ 0.577,\ 0.577,\ 0.577)$, $\mu_1 = 1.646 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 1.000,\ 0.000)$, $\mu_2 = 0.671 \times 10^{12}$
$\hat{q}^3 = (-0.786,-0.437,-0.437)$, $\hat{P}^3 = (-0.693,\ 0.509,\ 0.509)$, $\mu_3 = 0.470 \times 10^{12}$
$\omega_2/\omega_1 = -0.294$, $\omega_3/\omega_1 = 0.706$, $G = +0.181C_{144} - 0.150C_{166} + 0.362C_{456} + 0.470 \times 10^{12}$

Interaction Number 17

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.671 \times 10^{12}$
$\hat{q}^2 = (\ 0.958,-0.287,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.671 \times 10^{12}$
$\hat{q}^3 = (\ 0.511,\ 0.860,\ 0.000)$, $\hat{P}^3 = (\ 0.800,-0.600,\ 0.000)$, $\mu_3 = 0.452 \times 10^{12}$
$\omega_2/\omega_1 = -0.255$, $\omega_3/\omega_1 = 0.745$, $G = -0.432C_{144} + 0.381C_{166} + 0.181C_{456} + 0.404 \times 10^{12}$

Interaction Number 18

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.671 \times 10^{12}$
$\hat{q}^2 = (\ 0.894,\ 0.447,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.671 \times 10^{12}$
$\hat{q}^3 = (\ 0.399,\ 0.917,\ 0.000)$, $\hat{P}^3 = (\ 0.850,-0.526,\ 0.000)$, $\mu_3 = 0.508 \times 10^{12}$
$\omega_2/\omega_1 = -0.571$, $\omega_3/\omega_1 = 0.429$, $G = -0.198C_{144} + 0.062C_{166} + 0.541C_{456} + 0.347 \times 10^{12}$

Interaction Number 19

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.671 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.492 \times 10^{12}$
$\hat{q}^3 = (\ 0.705,\ 0.705,-0.076)$, $\hat{P}^3 = (-0.707,\ 0.707,\ 0.000)$, $\mu_3 = 0.405 \times 10^{12}$
$\omega_2/\omega_1 = -0.127$, $\omega_3/\omega_1 = 0.873$, $G = -0.319C_{144} + 0.319C_{166} + 0.428 \times 10^{12}$

Table 16. Useful Interactions for Silicon. Values of the second order constants used here are:

$C_{11} = 1.657 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.796 \times 10^{12}$ dyn/cm^2, $C_{12} = 0.639 \times 10^{12}$ dyn/cm^2.

Interaction Number 1

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.796 \times 10^{12}$
$\hat{q}^2 = (-0.707, 0.707, 0.000)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 1.944 \times 10^{12}$
$\hat{q}^3 = (0.989, 0.145, 0.000)$, $\hat{P}^3 = (0.973, 0.230, 0.000)$, $\mu_3 = 1.688 \times 10^{12}$
$\omega_2/\omega_1 = 0.283$, $\omega_3/\omega_1 = 1.283$, $G = -0.628C_{166} - 0.677 \times 10^{12}$

Interaction Number 2

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.796 \times 10^{12}$
$\hat{q}^2 = (0.000, 1.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 1.657 \times 10^{12}$
$\hat{q}^3 = (0.903, 0.429, 0.000)$, $\hat{P}^3 = (0.848, 0.529, 0.000)$, $\mu_3 = 1.846 \times 10^{12}$
$\omega_2/\omega_1 = 0.685$, $\omega_3/\omega_1 = 1.686$, $G = +0.842C_{166} + 1.357 \times 10^{12}$

Interaction Number 3

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.796 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.796 \times 10^{12}$
$\hat{q}^3 = (0.489, 0.873, 0.000)$, $\hat{P}^3 = (0.820, -0.572, 0.000)$, $\mu_3 = 0.575 \times 10^{12}$
$\omega_2/\omega_1 = -0.311$, $\omega_3/\omega_1 = 0.689$, $G = -0.353C_{144} + 0.283C_{166} + 0.308C_{456} + 0.489 \times 10^{12}$

Interaction Number 4

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.509 \times 10^{12}$
$\hat{q}^2 = (0.447, -0.894, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.796 \times 10^{12}$
$\hat{q}^3 = (0.811, 0.586, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.796 \times 10^{12}$
$\omega_2/\omega_1 = 0.202$, $\omega_3/\omega_1 = 1.202$, $G = +0.443C_{144} - 0.443C_{166} - 0.451 \times 10^{12}$

Table 16. (Continued)

Interaction Number 5

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.509 \times 10^{12}$
$\hat{q}^2 = (0.707, -0.707, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.796 \times 10^{12}$
$\hat{q}^3 = (0.845, 0.535, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.796 \times 10^{12}$
$\omega_2/\omega_1 = 0.281$, $\omega_3/\omega_1 = 1.282$, $G = +0.488C_{144} - 0.488C_{166} - 0.497 \times 10^{12}$

Interaction Number 6

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (1.000, 0.000, 0.000)$, $\mu_1 = 1.657 \times 10^{12}$
$\hat{q}^2 = (0.577, 0.577, 0.577)$, $\hat{P}^2 = (-0.408, -0.408, 0.816)$, $\mu_2 = 0.605 \times 10^{12}$
$\hat{q}^3 = (0.641, -0.543, -0.543)$, $\hat{P}^3 = (0.000, -0.707, 0.707)$, $\mu_3 = 0.627 \times 10^{12}$
$\omega_2/\omega_1 = -0.480$, $\omega_3/\omega_1 = 0.520$, $G = -0.271C_{112} + 0.320C_{166} + 0.271C_{123} + 0.184 \times 10^{12}$

Interaction Number 7

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.707, 0.707, 0.000)$, $\mu_1 = 1.944 \times 10^{12}$
$\hat{q}^2 = (-0.577, 0.577, 0.577)$, $\hat{P}^2 = (0.707, 0.707, 0.000)$, $\mu_2 = 0.605 \times 10^{12}$
$\hat{q}^3 = (0.903, 0.313, -0.295)$, $\hat{P}^3 = (-0.547, 0.629, -0.553)$, $\mu_3 = 0.644 \times 10^{12}$
$\omega_2/\omega_1 = -0.331$, $\omega_3/\omega_1 = 0.669$, $G = +0.141C_{111} - 0.141C_{112} - 0.142C_{144} - 0.142C_{166} - 0.285C_{456} + 0.029 \times 10^{12}$

Interaction Number 8

$\hat{q}^1 = (-0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 1.944 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (1.000, 0.000, 0.000)$, $\mu_2 = 1.657 \times 10^{12}$
$\hat{q}^3 = (-0.832, 0.555, 0.000)$, $\hat{P}^3 = (0.616, 0.788, 0.000)$, $\mu_3 = 0.544 \times 10^{12}$
$\omega_2/\omega_1 = -0.326$, $\omega_3/\omega_1 = 0.674$, $G = -0.256C_{111} + 0.181C_{112} + 0.314C_{166} - 0.870 \times 10^{12}$

Interaction Number 9

$\hat{q}^1 = (-0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 1.944 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.796 \times 10^{12}$
$\hat{q}^3 = (-0.823, 0.568, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.796 \times 10^{12}$
$\omega_2/\omega_1 = -0.203$, $\omega_3/\omega_1 = 0.797$, $G = -0.412C_{144} - 0.412C_{166} - 0.568C_{456} - 1.397 \times 10^{12}$

Table 16. (Continued)

Interaction Number 10

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.796 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.605 \times 10^{12}$
$\hat{q}^3 = (\ 0.705,\ 0.705,-0.067)$, $\hat{P}^3 = (-0.707,\ 0.707,\ 0.000)$, $\mu_3 = 0.510 \times 10^{12}$
$\omega_2/\omega_1 = -0.113$, $\omega_3/\omega_1 = 0.887$, $G = -0.316C_{144} + 0.316C_{166} + 0.502 \times 10^{12}$

Interaction Number 11

$\hat{q}^1 = (-0.577,-0.577,-0.577)$, $\hat{P}^1 = (\ 0.577,\ 0.577,\ 0.577)$, $\mu_1 = 2.040 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 1.000,\ 0.000)$, $\mu_2 = 0.796 \times 10^{12}$
$\hat{q}^3 = (-0.772,-0.450,-0.450)$, $\hat{P}^3 = (\ 0.000,-0.707,\ 0.707)$, $\mu_3 = 0.680 \times 10^{12}$
$\omega_2/\omega_1 = -0.258$, $\omega_3/\omega_1 = 0.741$, $G = +0.030C_{144} - 0.576C_{166} + 0.364C_{456} - 0.871 \times 10^{12}$

Interaction Number 12

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.509 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.605 \times 10^{12}$
$\hat{q}^3 = (\ 0.705,\ 0.705,\ 0.075)$, $\hat{P}^3 = (-0.066,-0.066,\ 0.996)$, $\mu_3 = 0.791 \times 10^{12}$
$\omega_2/\omega_1 = 0.129$, $\omega_3/\omega_1 = 1.129$, $G = +0.019C_{111} - 0.050C_{112} - 0.285C_{144} + 0.285C_{166} + 0.031C_{123} + 0.562 \times 10^{12}$

Interaction Number 13

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.796 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (\ 0.577,\ 0.577,-0.577)$, $\mu_2 = 2.040 \times 10^{12}$
$\hat{q}^3 = (\ 0.700,\ 0.700,\ 0.138)$, $\hat{P}^3 = (\ 0.697,\ 0.697,\ 0.169)$, $\mu_3 = 1.956 \times 10^{12}$
$\omega_2/\omega_1 = 0.322$, $\omega_3/\omega_1 = 1.323$, $G = +0.359C_{144} + 0.280C_{166} + 0.719C_{456} + 0.845 \times 10^{12}$

Interaction Number 14

$\hat{q}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\mu_1 = 1.657 \times 10^{12}$
$\hat{q}^2 = (\ 0.577,\ 0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.605 \times 10^{12}$
$\hat{q}^3 = (\ 0.641,-0.543,-0.543)$, $\hat{P}^3 = (\ 0.000,-0.707,\ 0.707)$, $\mu_3 = 0.627 \times 10^{12}$
$\omega_2/\omega_1 = -0.480$, $\omega_3/\omega_1 = 0.520$, $G = +0.157C_{112} - 0.185C_{166} - 0.157C_{123} - 0.106 \times 10^{12}$

Table 16. (Continued)

Interaction Number 15

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.707, 0.707, 0.000)$, $\mu_1 = 1.944 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.605 \times 10^{12}$
$\hat{q}^3 = (0.694, 0.694,-0.195)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.520 \times 10^{12}$
$\omega_2/\omega_1 = -0.267$, $\omega_3/\omega_1 = 0.733$, $G = -0.200C_{111} +0.200C_{112} -0.056C_{144} -0.056C_{166} +0.113C_{456} -1.629 \times 10^{12}$

Interaction Number 16

$\hat{q}^1 = (-0.577,-0.577,-0.577)$, $\hat{P}^1 = (0.577, 0.577, 0.577)$, $\mu_1 = 2.040 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 0.796 \times 10^{12}$
$\hat{q}^3 = (-0.788,-0.436,-0.436)$, $\hat{P}^3 = (-0.682, 0.517, 0.517)$, $\mu_3 = 0.583 \times 10^{12}$
$\omega_2/\omega_1 = -0.291$, $\omega_3/\omega_1 = 0.708$, $G = +0.187C_{144} -0.134C_{166} +0.374C_{456} +0.610 \times 10^{12}$

Interaction Number 17

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.796 \times 10^{12}$
$\hat{q}^2 = (0.958,-0.287, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.796 \times 10^{12}$
$\hat{q}^3 = (0.525, 0.851, 0.000)$, $\hat{P}^3 = (0.802,-0.597, 0.000)$, $\mu_3 = 0.557 \times 10^{12}$
$\omega_2/\omega_1 = -0.238$, $\omega_3/\omega_1 = 0.762$, $G = -0.430C_{144} +0.389C_{166} +0.175C_{456} +0.509 \times 10^{12}$

Interaction Number 18

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.796 \times 10^{12}$
$\hat{q}^2 = (0.894, 0.447, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.796 \times 10^{12}$
$\hat{q}^3 = (0.415, 0.910, 0.000)$, $\hat{P}^3 = (0.855,-0.519, 0.000)$, $\mu_3 = 0.616 \times 10^{12}$
$\omega_2/\omega_1 = -0.557$, $\omega_3/\omega_1 = 0.443$, $G = -0.186C_{144} +0.075C_{166} +0.534C_{456} +0.430 \times 10^{12}$

Interaction Number 19

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.796 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.605 \times 10^{12}$
$\hat{q}^3 = (0.705, 0.705,-0.067)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.510 \times 10^{12}$
$\omega_2/\omega_1 = -0.113$, $\omega_3/\omega_1 = 0.887$, $G = -0.316C_{144} +0.316C_{166} +0.502 \times 10^{12}$

Table 17. Useful Interactions for Potassium Chloride. Values of the second order constants used here are:

$C_{11} = 0.398 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.00625 \times 10^{12}$ dyn/cm^2, $C_{12} = 0.062 \times 10^{12}$ dyn/cm^2.

Interaction Number 1

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.006 \times 10^{12}$
$\hat{q}^2 = (-0.707, 0.707, 0.000)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.236 \times 10^{12}$
$\hat{q}^3 = (0.805, 0.593, 0.000)$, $\hat{P}^3 = (0.967, 0.253, 0.000)$, $\mu_3 = 0.269 \times 10^{12}$
$\omega_2/\omega_1 = 3.689$, $\omega_3/\omega_1 = 4.689$, $G = -0.151C_{166} - 0.112 \times 10^{12}$

Interaction Number 2

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.168 \times 10^{12}$
$\hat{q}^2 = (0.447,-0.894, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.006 \times 10^{12}$
$\hat{q}^3 = (-0.122, 0.993, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.006 \times 10^{12}$
$\omega_2/\omega_1 = -0.454$, $\omega_3/\omega_1 = 0.546$, $G = +0.417C_{144} - 0.417C_{166} - 0.140 \times 10^{12}$

Interaction Number 3

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.168 \times 10^{12}$
$\hat{q}^2 = (0.707,-0.707, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.006 \times 10^{12}$
$\hat{q}^3 = (-0.393, 0.919, 0.000)$, $\hat{P}^3 = (0.000, 0.000, 1.000)$, $\mu_3 = 0.006 \times 10^{12}$
$\omega_2/\omega_1 = -0.481$, $\omega_3/\omega_1 = 0.518$, $G = +0.186C_{144} - 0.186C_{166} - 0.063 \times 10^{12}$

Interaction Number 4

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (1.000, 0.000, 0.000)$, $\mu_1 = 0.398 \times 10^{12}$
$\hat{q}^2 = (0.577, 0.577, 0.577)$, $\hat{P}^2 = (-0.408,-0.408, 0.816)$, $\mu_2 = 0.114 \times 10^{12}$
$\hat{q}^3 = (0.516,-0.606,-0.606)$, $\hat{P}^3 = (0.000,-0.707, 0.707)$, $\mu_3 = 0.125 \times 10^{12}$
$\omega_2/\omega_1 = -0.500$, $\omega_3/\omega_1 = 0.499$, $G = -0.303C_{112} + 0.258C_{166} + 0.303C_{123} + 0.065 \times 10^{12}$

Table 17. (Continued)

Interaction Number 5

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.236 \times 10^{12}$
$\hat{q}^2 = (-0.577,\ 0.577,\ 0.577)$, $\hat{P}^2 = (\ 0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.114 \times 10^{12}$
$\hat{q}^3 = (\ 0.909,\ 0.267,-0.321)$, $\hat{P}^3 = (\ 0.085,-0.323,\ 0.943)$, $\mu_3 = 0.047 \times 10^{12}$
$\omega_2/\omega_1 = -0.465$, $\omega_3/\omega_1 = 0.536$, $G = -0.033C_{111} + 0.033C_{112} + 0.242C_{144} + 0.242C_{166} + 0.483C_{456} + 0.007 \times 10^{12}$

Interaction Number 6

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.168 \times 10^{12}$
$\hat{q}^2 = (\ 0.577,\ 0.577,\ 0.577)$, $\hat{P}^2 = (-0.408,-0.408,\ 0.816)$, $\mu_2 = 0.114 \times 10^{12}$
$\hat{q}^3 = (\ 0.707,\ 0.707,-0.033)$, $\hat{P}^3 = (-0.707,\ 0.707,\ 0.000)$, $\mu_3 = 0.168 \times 10^{12}$
$\omega_2/\omega_1 = -0.045$, $\omega_3/\omega_1 = 0.955$, $G = -0.118C_{111} + 0.353C_{112} + 0.005C_{144} - 0.005C_{166} - 0.236C_{123} - 0.082 \times 10^{12}$

Interaction Number 7

$\hat{q}^1 = (-0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.236 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\mu_2 = 0.398 \times 10^{12}$
$\hat{q}^3 = (-0.749,\ 0.662,\ 0.000)$, $\hat{P}^3 = (\ 0.459,\ 0.888,\ 0.000)$, $\mu_3 = 0.161 \times 10^{12}$
$\omega_2/\omega_1 = -0.120$, $\omega_3/\omega_1 = 0.880$, $G = -0.172C_{111} + 0.416C_{112} + 0.361C_{166} - 0.057 \times 10^{12}$

Interaction Number 8

$\hat{q}^1 = (-0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.236 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.006 \times 10^{12}$
$\hat{q}^3 = (-0.979,\ 0.204,\ 0.000)$, $\hat{P}^3 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_3 = 0.006 \times 10^{12}$
$\omega_2/\omega_1 = -0.436$, $\omega_3/\omega_1 = 0.563$, $G = -0.489C_{144} - 0.489C_{166} - 0.204C_{456} - 0.226 \times 10^{12}$

Interaction Number 9

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.006 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.114 \times 10^{12}$
$\hat{q}^3 = (\ 0.638,\ 0.638,\ 0.431)$, $\hat{P}^3 = (-0.707,\ 0.707,\ 0.000)$, $\mu_3 = 0.138 \times 10^{12}$
$\omega_2/\omega_1 = 2.108$, $\omega_3/\omega_1 = 3.109$, $G = -0.085C_{144} + 0.085C_{166} + 0.001 \times 10^{12}$

Table 17. (Continued)

Interaction Number 10

$\hat{q}^1 = (-0.577,-0.577,-0.577)$, $\hat{P}^1 = (0.577, 0.577, 0.577)$, $\mu_1 = 0.182 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 0.006 \times 10^{12}$
$\hat{q}^3 = (-0.877,-0.340,-0.340)$, $\hat{P}^3 = (0.000,-0.707, 0.707)$, $\mu_3 = 0.044 \times 10^{12}$
$\omega_2/\omega_1 = -0.169$, $\omega_3/\omega_1 = 0.831$, $G = -0.046C_{144} - 0.574C_{166} + 0.413C_{456} - 0.110 \times 10^{12}$

Interaction Number 11

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.168 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.114 \times 10^{12}$
$\hat{q}^3 = (0.691, 0.691,-0.213)$, $\hat{P}^3 = (0.049, 0.049, 0.998)$, $\mu_3 = 0.023 \times 10^{12}$
$\omega_2/\omega_1 = -0.451$, $\omega_3/\omega_1 = 0.549$, $G = -0.014C_{111} + 0.101C_{112} - 0.277C_{144} + 0.277C_{166}$
$-0.087C_{123} + 0.001 \times 10^{12}$

Interaction Number 12

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.006 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (0.577, 0.577,-0.577)$, $\mu_2 = 0.182 \times 10^{12}$
$\hat{q}^3 = (0.635, 0.635, 0.439)$, $\hat{P}^3 = (0.689, 0.689, 0.226)$, $\mu_3 = 0.198 \times 10^{12}$
$\omega_2/\omega_1 = 2.705$, $\omega_3/\omega_1 = 3.705$, $G = +0.202C_{144} + 0.086C_{166} + 0.405C_{456} + 0.064 \times 10^{12}$

Interaction Number 13

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (1.000, 0.000, 0.000)$, $\mu_1 = 0.398 \times 10^{12}$
$\hat{q}^2 = (0.577, 0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.114 \times 10^{12}$
$\hat{q}^3 = (0.516,-0.606,-0.606)$, $\hat{P}^3 = (0.000,-0.707, 0.707)$, $\mu_3 = 0.125 \times 10^{12}$
$\omega_2/\omega_1 = -0.501$, $\omega_3/\omega_1 = 0.499$, $G = +0.175C_{112} - 0.149C_{166} - 0.175C_{123} - 0.038 \times 10^{12}$

Interaction Number 14

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.707, 0.707, 0.000)$, $\mu_1 = 0.236 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.114 \times 10^{12}$
$\hat{q}^3 = (0.706, 0.706,-0.060)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.167 \times 10^{12}$
$\omega_2/\omega_1 = -0.079$, $\omega_3/\omega_1 = 0.921$, $G = -0.204C_{111} + 0.204C_{112} - 0.017C_{144} - 0.017C_{166}$
$+0.035C_{456} - 0.195 \times 10^{12}$

Table 17. (Continued)

Interaction Number 15

$\hat{q}^1 = (-0.577,-0.577,-0.577)$, $\hat{P}^1 = (0.577, 0.577, 0.577)$, $\mu_1 = 0.182 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 0.006 \times 10^{12}$
$\hat{q}^3 = (-0.786,-0.437,-0.437)$, $\hat{P}^3 = (-0.201, 0.693, 0.693)$, $\mu_3 = 0.087 \times 10^{12}$
$\omega_2/\omega_1 = -0.086$, $\omega_3/\omega_1 = 0.914$, $G = +0.354C_{144} +0.401C_{166} +0.708C_{456} +0.094 \times 10^{12}$

Interaction Number 16

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.006 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.114 \times 10^{12}$
$\hat{q}^3 = (0.638, 0.638, 0.431)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.138 \times 10^{12}$
$\omega_2/\omega_1 = 2.108$, $\omega_3/\omega_1 = 3.109$, $G = -0.085C_{144} +0.085C_{166} +0.001 \times 10^{12}$

Interaction Number 17

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.006 \times 10^{12}$
$\hat{q}^2 = (-0.894, 0.447, 0.000)$, $\hat{P}^2 = (0.993,-0.114, 0.000)$, $\mu_2 = 0.323 \times 10^{12}$
$\hat{q}^3 = (0.932, 0.362, 0.000)$, $\hat{P}^3 = (0.997, 0.079, 0.000)$, $\mu_3 = 0.349 \times 10^{12}$
$\omega_2/\omega_1 = 3.510$, $\omega_3/\omega_1 = 4.511$, $G = +0.115C_{166} +0.012 \times 10^{12}$

Table 18. Useful Interactions for Sodium Chloride. Values of the second order constants used here are:

$C_{11} = 0.487 \times 10^{12}$ dyn/cm^2, $C_{44} = 0.126 \times 10^{12}$ dyn/cm^2, $C_{12} = 0.124 \times 10^{12}$ dyn/cm^2.

Interaction Number 1

$\hat{q}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 1.000,\ 0.000)$, $\mu_1 = 0.126 \times 10^{12}$
$\hat{q}^2 = (-0.707,\ 0.707,\ 0.000)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.432 \times 10^{12}$
$\hat{q}^3 = (\ 0.963,\ 0.270,\ 0.000)$, $\hat{P}^3 = (\ 0.980,\ 0.198,\ 0.000)$, $\mu_3 = 0.474 \times 10^{12}$
$\omega_2/\omega_1 = 0.573$, $\omega_3/\omega_1 = 1.573$, $G = -0.542C_{166} - 0.187 \times 10^{12}$

Interaction Number 2

$\hat{q}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 1.000,\ 0.000)$, $\mu_1 = 0.126 \times 10^{12}$
$\hat{q}^2 = (\ 0.000,\ 1.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 1.000,\ 0.000)$, $\mu_2 = 0.487 \times 10^{12}$
$\hat{q}^3 = (\ 0.853,\ 0.522,\ 0.000)$, $\hat{P}^3 = (\ 0.893,\ 0.450,\ 0.000)$, $\mu_3 = 0.445 \times 10^{12}$
$\omega_2/\omega_1 = 1.202$, $\omega_3/\omega_1 = 2.203$, $G = +0.850C_{166} + 0.203 \times 10^{12}$

Interaction Number 3

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.126 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.126 \times 10^{12}$
$\hat{q}^3 = (\ 0.937,\ 0.350,\ 0.000)$, $\hat{P}^3 = (-0.268,\ 0.964,\ 0.000)$, $\mu_3 = 0.147 \times 10^{12}$
$\omega_2/\omega_1 = 1.185$, $\omega_3/\omega_1 = 2.185$, $G = +0.239C_{144} - 0.177C_{166} + 0.572C_{456} + 0.015 \times 10^{12}$

Interaction Number 4

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.182 \times 10^{12}$
$\hat{q}^2 = (\ 0.447,-0.894,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.126 \times 10^{12}$
$\hat{q}^3 = (\ 0.609,\ 0.793,\ 0.000)$, $\hat{P}^3 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_3 = 0.126 \times 10^{12}$
$\omega_2/\omega_1 = -0.121$, $\omega_3/\omega_1 = 0.879$, $G = +0.491C_{144} - 0.491C_{166} - 0.178 \times 10^{12}$

Table 18. (Continued)

Interaction Number 5

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.182 \times 10^{12}$
$\hat{q}^2 = (\ 0.707, -0.707,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.126 \times 10^{12}$
$\hat{q}^3 = (\ 0.568,\ 0.823,\ 0.000)$, $\hat{P}^3 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_3 = 0.126 \times 10^{12}$
$\omega_2/\omega_1 = -0.153$, $\omega_3/\omega_1 = 0.847$, $G = +0.492C_{144} - 0.492C_{166} - 0.179 \times 10^{12}$

Interaction Number 6

$\hat{q}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^1 = (\ 1.000,\ 0.000,\ 0.000)$, $\mu_1 = 0.487 \times 10^{12}$
$\hat{q}^2 = (\ 0.577,\ 0.577,\ 0.577)$, $\hat{P}^2 = (-0.408, -0.408,\ 0.816)$, $\mu_2 = 0.163 \times 10^{12}$
$\hat{q}^3 = (\ 0.580, -0.576, -0.576)$, $\hat{P}^3 = (\ 0.000, -0.707,\ 0.707)$, $\mu_3 = 0.163 \times 10^{12}$
$\omega_2/\omega_1 = -0.499$, $\omega_3/\omega_1 = 0.500$, $G = -0.288C_{112} + 0.290C_{166} + 0.288C_{123} + 0.070 \times 10^{12}$

Interaction Number 7

$\hat{q}^1 = (-0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.432 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\mu_2 = 0.487 \times 10^{12}$
$\hat{q}^3 = (-0.799,\ 0.601,\ 0.000)$, $\hat{P}^3 = (\ 0.555,\ 0.832,\ 0.000)$, $\mu_3 = 0.176 \times 10^{12}$
$\omega_2/\omega_1 = -0.248$, $\omega_3/\omega_1 = 0.752$, $G = -0.222C_{111} + 0.279C_{112} + 0.332C_{166} - 0.169 \times 10^{12}$

Interaction Number 8

$\hat{q}^1 = (-0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (-0.707,\ 0.707,\ 0.000)$, $\mu_1 = 0.432 \times 10^{12}$
$\hat{q}^2 = (\ 1.000,\ 0.000,\ 0.000)$, $\hat{P}^2 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_2 = 0.126 \times 10^{12}$
$\hat{q}^3 = (-0.858,\ 0.514,\ 0.000)$, $\hat{P}^3 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_3 = 0.126 \times 10^{12}$
$\omega_2/\omega_1 = -0.256$, $\omega_3/\omega_1 = 0.744$, $G = -0.429C_{144} - 0.429C_{166} - 0.514C_{456} - 0.327 \times 10^{12}$

Interaction Number 9

$\hat{q}^1 = (\ 0.707,\ 0.707,\ 0.000)$, $\hat{P}^1 = (\ 0.000,\ 0.000,\ 1.000)$, $\mu_1 = 0.126 \times 10^{12}$
$\hat{q}^2 = (-0.577, -0.577,\ 0.577)$, $\hat{P}^2 = (-0.707,\ 0.707,\ 0.000)$, $\mu_2 = 0.163 \times 10^{12}$
$\hat{q}^3 = (\ 0.706,\ 0.706,\ 0.059)$, $\hat{P}^3 = (-0.707,\ 0.707,\ 0.000)$, $\mu_3 = 0.181 \times 10^{12}$
$\omega_2/\omega_1 = 0.108$, $\omega_3/\omega_1 = 1.108$, $G = -0.264C_{144} + 0.264C_{166} + 0.067 \times 10^{12}$

Table 18. (Continued)

Interaction Number 10

$\hat{q}^1 = (-0.577,-0.577,-0.577)$, $\hat{P}^1 = (0.577, 0.577, 0.577)$, $\mu_1 = 0.413 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 0.126 \times 10^{12}$
$\hat{q}^3 = (-0.772,-0.449,-0.449)$, $\hat{P}^3 = (0.000,-0.707, 0.707)$, $\mu_3 = 0.148 \times 10^{12}$
$\omega_2/\omega_1 = -0.229$, $\omega_3/\omega_1 = 0.770$, $G = +0.030C_{144} -0.576C_{166} +0.364C_{456} -0.187 \times 10^{12}$

Interaction Number 11

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (-0.707, 0.707, 0.000)$, $\mu_1 = 0.182 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.163 \times 10^{12}$
$\hat{q}^3 = (0.706, 0.706,-0.054)$, $\hat{P}^3 = (0.031, 0.031, 0.999)$, $\mu_3 = 0.126 \times 10^{12}$
$\omega_2/\omega_1 = -0.096$, $\omega_3/\omega_1 = 0.905$, $G = -0.009C_{111} +0.031C_{112} -0.287C_{144} +0.287C_{166}$
$-0.022C_{123} +0.062 \times 10^{12}$

Interaction Number 12

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.126 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (0.577, 0.577,-0.577)$, $\mu_2 = 0.413 \times 10^{12}$
$\hat{q}^3 = (0.694, 0.694, 0.189)$, $\hat{P}^3 = (0.698, 0.698, 0.159)$, $\mu_3 = 0.428 \times 10^{12}$
$\omega_2/\omega_1 = 0.475$, $\omega_3/\omega_1 = 1.475$, $G = +0.343C_{144} +0.257C_{166} +0.686C_{456} +0.174 \times 10^{12}$

Interaction Number 13

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (1.000, 0.000, 0.000)$, $\mu_1 = 0.487 \times 10^{12}$
$\hat{q}^2 = (0.577, 0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.163 \times 10^{12}$
$\hat{q}^3 = (0.580,-0.576,-0.576)$, $\hat{P}^3 = (0.000,-0.707, 0.707)$, $\mu_3 = 0.163 \times 10^{12}$
$\omega_2/\omega_1 = -0.499$, $\omega_3/\omega_1 = 0.500$, $G = +0.166C_{112} -0.167C_{166} -0.166C_{123} -0.040 \times 10^{12}$

Interaction Number 14

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.707, 0.707, 0.000)$, $\mu_1 = 0.432 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.163 \times 10^{12}$
$\hat{q}^3 = (0.700, 0.700,-0.139)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.180 \times 10^{12}$
$\omega_2/\omega_1 = -0.186$, $\omega_3/\omega_1 = 0.814$, $G = -0.202C_{111} +0.202C_{112} -0.040C_{144} -0.040C_{166}$
$+0.080C_{456} -0.359 \times 10^{12}$

Table 18. (Continued)

Interaction Number 15

$\hat{q}^1 = (-0.577,-0.577,-0.577)$, $\hat{P}^1 = (0.577, 0.577, 0.577)$, $\mu_1 = 0.413 \times 10^{12}$
$\hat{q}^2 = (1.000, 0.000, 0.000)$, $\hat{P}^2 = (0.000, 1.000, 0.000)$, $\mu_2 = 0.126 \times 10^{12}$
$\hat{q}^3 = (-0.759,-0.460,-0.460)$, $\hat{P}^3 = (-0.591, 0.571, 0.571)$, $\mu_3 = 0.165 \times 10^{12}$
$\omega_2/\omega_1 = -0.207$, $\omega_3/\omega_1 = 0.793$, $G = +0.229C_{144} -0.016C_{166} +0.458C_{456} +0.141 \times 10^{12}$

Interaction Number 16

$\hat{q}^1 = (1.000, 0.000, 0.000)$, $\hat{P}^1 = (0.000, 1.000, 0.000)$, $\mu_1 = 0.126 \times 10^{12}$
$\hat{q}^2 = (-0.229, 0.688, 0.688)$, $\hat{P}^2 = (-0.195, 0.694, 0.694)$, $\mu_2 = 0.426 \times 10^{12}$
$\hat{q}^3 = (0.881, 0.335, 0.335)$, $\hat{P}^3 = (0.925, 0.268, 0.268)$, $\mu_3 = 0.449 \times 10^{12}$
$\omega_2/\omega_1 = 0.901$, $\omega_3/\omega_1 = 1.902$, $G = +0.234C_{144} +0.020C_{166} +0.469C_{456} +0.038 \times 10^{12}$

Interaction Number 17

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.126 \times 10^{12}$
$\hat{q}^2 = (0.958,-0.287, 0.000)$, $\hat{P}^2 = (0.000, 0.000, 1.000)$, $\mu_2 = 0.126 \times 10^{12}$
$\hat{q}^3 = (0.885, 0.466, 0.000)$, $\hat{P}^3 = (-0.385, 0.923, 0.000)$, $\mu_3 = 0.161 \times 10^{12}$
$\omega_2/\omega_1 = 0.423$, $\omega_3/\omega_1 = 1.423$, $G = +0.360C_{144} -0.318C_{166} +0.302C_{456} -0.072 \times 10^{12}$

Interaction Number 18

$\hat{q}^1 = (0.707, 0.707, 0.000)$, $\hat{P}^1 = (0.000, 0.000, 1.000)$, $\mu_1 = 0.126 \times 10^{12}$
$\hat{q}^2 = (-0.577,-0.577, 0.577)$, $\hat{P}^2 = (-0.707, 0.707, 0.000)$, $\mu_2 = 0.163 \times 10^{12}$
$\hat{q}^3 = (0.706, 0.706, 0.059)$, $\hat{P}^3 = (-0.707, 0.707, 0.000)$, $\mu_3 = 0.181 \times 10^{12}$
$\omega_2/\omega_1 = 0.108$, $\omega_3/\omega_1 = 1.108$, $G = -0.264C_{144} +0.264C_{166} +0.067 \times 10^{12}$

Table 19. Values of Third Order Elastic Constants for Copper

Elastic Constant	Value in dynes/cm^2
C_{111}	-12.71×10^{12}
C_{112}	-8.14×10^{12}
C_{123}	-0.50×10^{12}
C_{144}	-0.03×10^{12}
C_{166}	-7.80×10^{12}
C_{456}	-0.95×10^{12}

APPENDIX

The purpose of this appendix is to show, by means of a perturbation calculation, that the contribution of the non-resonant terms in Equation (24) can usually be neglected. To this end, Equation (24) is rewritten in the form

$$P_{j,aa} - \frac{\rho}{\mu_j} P_{j,tt} = - \frac{1}{\mu_j} \sum_{\ell,m=1}^{3} \nu_{j\ell m} P_{\ell,a} P_{m,aa} \quad , \tag{A-1}$$

where j takes on the values 1, 2, and 3 in this equation and in the next three equations. The symbols $P_{\ell,a}$, $P_{j,aa}$, and $P_{j,tt}$ are defined by the equations

$$P_{\ell,a} = \frac{\partial P_\ell}{\partial a} \quad ,$$

$$P_{j,aa} = \frac{\partial^2 P_j}{\partial a^2} \quad ,$$

and

$$P_{j,tt} = \frac{\partial^2 P_j}{\partial t^2} \quad .$$

To solve Equation (A-1), one notices that the terms on the right-hand side, the nonlinear terms, represent only a small perturbation of the homogeneous, uncoupled equations

$$P_{j,aa} - \frac{\rho}{\mu_j} P_{j,tt} = 0 \quad , \tag{A-2}$$

whose unperturbed solution is taken to be $P_j^\circ(a,t)$, a sinusoidal plane wave. The trial solution

$$P_j^T = P_j^\circ + P_j'(a,t) \tag{A-3}$$

is then substituted into Equation (A-1) and, by dropping second and higher order terms containing P_j' or its derivatives, one obtains the system of equations

$$P'_{j,aa} - \frac{\rho}{\mu_j} P'_{j,tt} = - \frac{1}{\mu_j} \sum_{\ell,m=1}^{3} \nu_{j\ell m} P^\circ_{\ell,a} P^\circ_{m,aa} \quad , \tag{A-4}$$

whose solution is the first order perturbation correction to the equations of motion. The terms on the right-hand side of Equation (A-4) are driving terms which depend on the choice of the initial solution, P_j°.

Since the partial differential equations represented by Equation (A-4) are linear and since they are not coupled in the dependent variables, one may concentrate his attention on the response of one of the components of P_j' to a single driving term. To do this, one now regards j as fixed and ignores all but one of the terms in the sum on the right-hand side of Equation (A-4). The new equation is

$$P'_{j,aa} - \frac{\rho}{\mu_j} P'_{j,tt} = - \frac{1}{\mu_j} \nu_{j\ell m} P^\circ_{\ell,a} P^\circ_{m,aa} \quad , \tag{A-5}$$

and its solution (32) is given by

$$P_j'(a,t) = - \frac{C_j}{2\mu_j} \int_o^t \int_{a-C_j(t-t')}^{a+C_j(t-t')} \nu_{j\ell m} P^\circ_{\ell,a}(a',t') P^\circ_{m,aa}(a',t') \, da' \, dt' \quad , \tag{A-6}$$

where the initial condition is $P'_j(a,0) = 0$ and the boundaries are taken at infinity. The quantity C_j is defined by the equation $C_j = \sqrt{\mu_j/\rho}$.

One would now like to use the solution given by Equation (A-6) to show the difference between the resonant and non-resonant terms and to indicate that the effect of the non-resonant terms can be neglected. This is accomplished by substituting the expressions

$$P^o_\ell = B_\ell \sin (\omega_\ell t + k_\ell a)$$

and

$$P^o_m = B_m \sin (\omega_m t + k_m a) \quad ,$$

which represent solutions to the unperturbed equations, Equation (A-2), into the integral of Equation (A-6). When this has been done, Equation (A-6) can be written as

$$P'_j(a,t) = + \frac{C_j}{2\mu_j} \nu_{j\ell m} B_\ell B_m k_\ell k_m^2 I \quad , \tag{A-7}$$

where the integral, I, can be written as the sum of two integrals,

$$I = I_S + I_D = \frac{1}{2} \int_o^t \int_{a-C_j(t-t')}^{a+C_j(t-t')} \sin (\omega_S t' + k_S ') \, da' \, dt' \tag{A-8}$$

$$+ \frac{1}{2} \int_o^t \int_{a-C_j(t-t')}^{a+C_j(t-t')} \sin (\omega_D t' + k_D a') \, da' \, dt' \quad ,$$

and the symbols ω_S, k_S, ω_D, and k_D are defined by the equations

$$\omega_S = \omega_\ell + \omega_m \quad ,$$

$$k_S = k_\ell + k_m \quad ,$$

$$\omega_D = \omega_m - \omega_\ell \quad ,$$

and

$$k_D = k_m - k_\ell \quad .$$

The integrals I_S and I_D contain the key to distinguishing between the resonant and non-resonant terms. Consider the contribution of I_S and assume for the moment that $k_S \neq 0$. If the resonance condition, $\omega_S \pm k_S C_j = 0$, is satisfied, then I_S will contribute a term of the form

$$T_R = \frac{1}{2k_S} t \cos(\omega_S t + k_S a) = \frac{a}{2k_S C_j} \cos(\omega_S t + k_S a) \qquad \text{(A-9)}$$

to the integral I. The other contributions of I_S will be of the non-resonant type,

$$T_{NR} = \frac{1}{2k_S} \cdot \left(\frac{1}{\omega_S - C_j k_S} \right) \left[\sin(\omega_S t + k_S a) - \sin(k_S a - C_j k_S t) \right] \quad . \qquad \text{(A-10)}$$

If no resonance condition is satisfied, then I_S will be composed entirely of non-resonant terms. To see that these non-resonant terms can be neglected, one needs to compare the amplitudes of the resonant and non-resonant terms given in Equations (A-9) and (A-10) for typical values of the parameters. If one takes $\omega_S - C_j k_S = 1.8 \times 10^7$ sec^{-1}, which is about 10 per cent of a typical frequency used in the experiment, and if

one supposes that a = 3 cm and $C_j = 5 \times 10^5$ cm/sec, then the ratio of the amplitudes will be 1.1×10^{-2}. Thus, the non-resonant terms can usually be neglected. Finally, one points out that if $k_S = 0$ then the contribution of I_S is even smaller than the non-resonant term given by Equation (A-10). This same discussion applies to the integral I_D, where the resonance condition would be $\omega_D \pm k_D C_j = 0$.

To conclude this appendix, one needs to show that the resonance conditions found in the above paragraph are equivalent to the ones given in the text of the thesis. To this end, notice that when the experiment is performed the initial wave is polarized along one of the independent polarization directions. Consequently, the driving terms in Equation (A-4) for which $\ell \neq m$ will vanish and need not be considered. Using $\ell = m$, the resonance conditions found in the preceding paragraph become

$$2\,\omega_\ell \pm 2\,k_\ell\,C_j = 0$$

which is equivalent to requiring that $C_j = \pm C_\ell$ and finally that $\mu_j = \mu_\ell$. This condition holds trivially if $j = \ell$.

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